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Hyper-polarized deuterium molecules: An option to produce and store polarized fuel for nuclear fusion?

23.07.2015

by Ralf Engels

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Polarized Fusion

Advantages of „polarized fuel“ for nuclear fusion are

undisputed since more than 40 years !

Why it was never used?

1.) Spin-dependence of the d-d reactions

2.) Conservation of the polarization in a plasma

3.) Production of polarized fuel, especialy deuterium

Outline

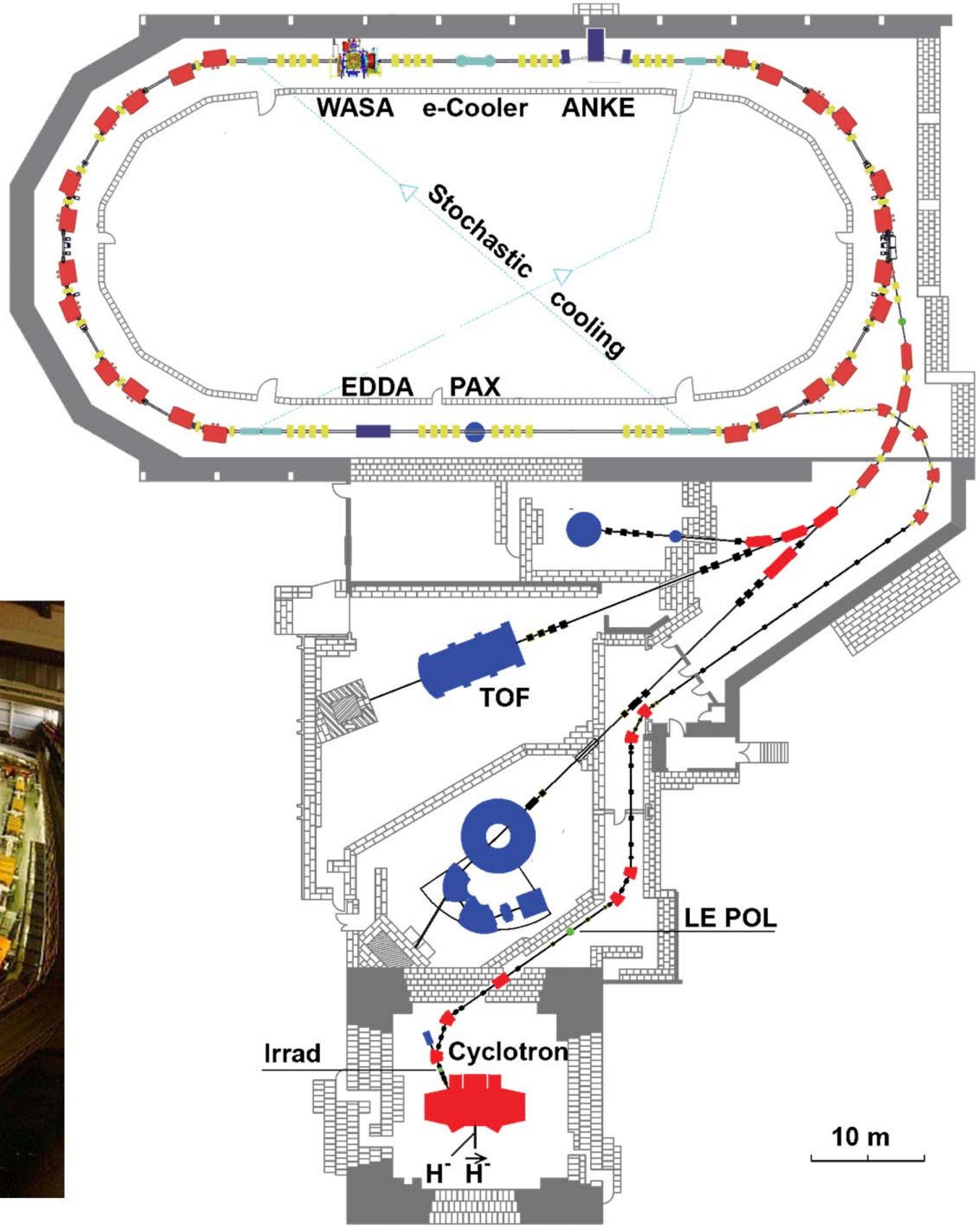
- Polarized Internal Targets in Nuclear Physics
- The experimental Setup
- Important Details about H_2/D_2 Molecules
- Expected Results
- Experimental Results
- Conclusion and Outlook

PIT@ANKE

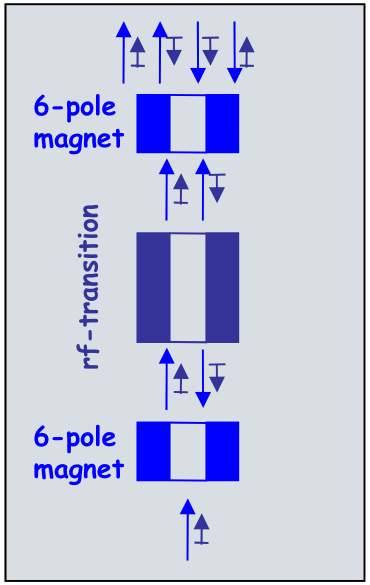
$$p, \vec{p}, d, \vec{d}$$

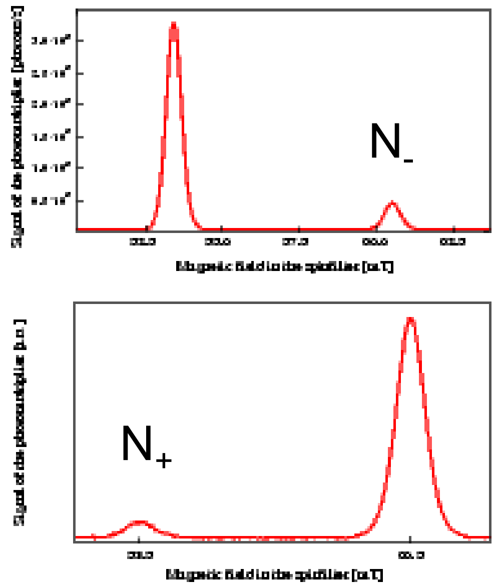
with momenta up to 3.7 GeV/c

- **internal experiments** – with the circulating beam
- **external experiments** – with the extracted beam

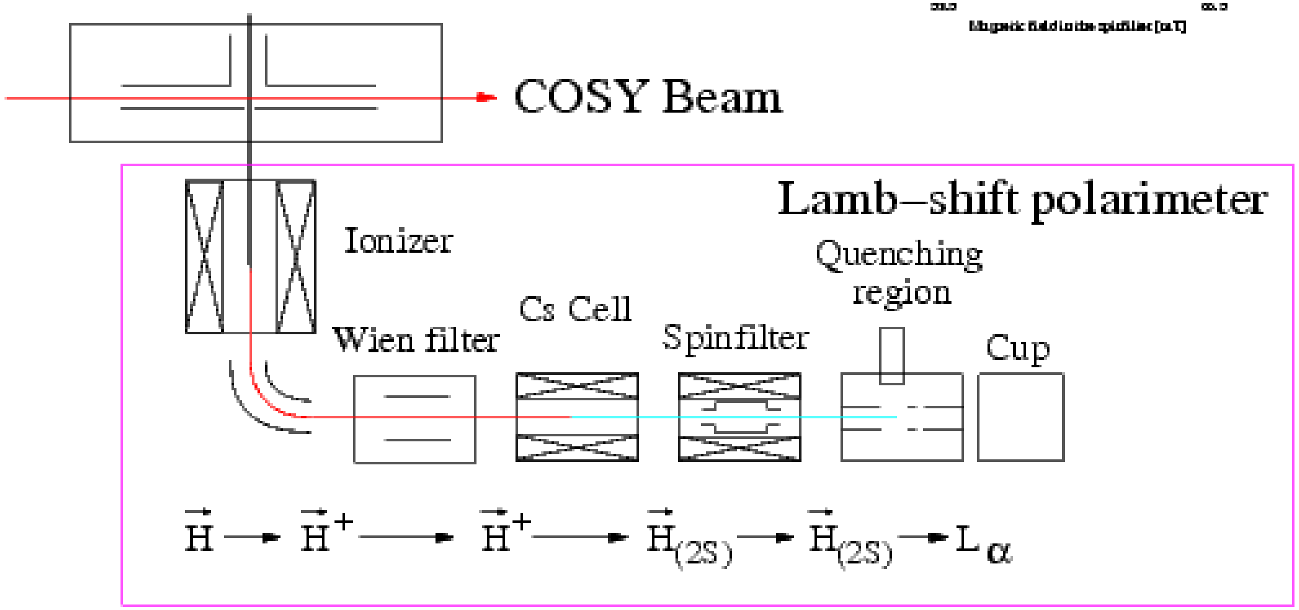


ABS and Lamb-shift polarimeter





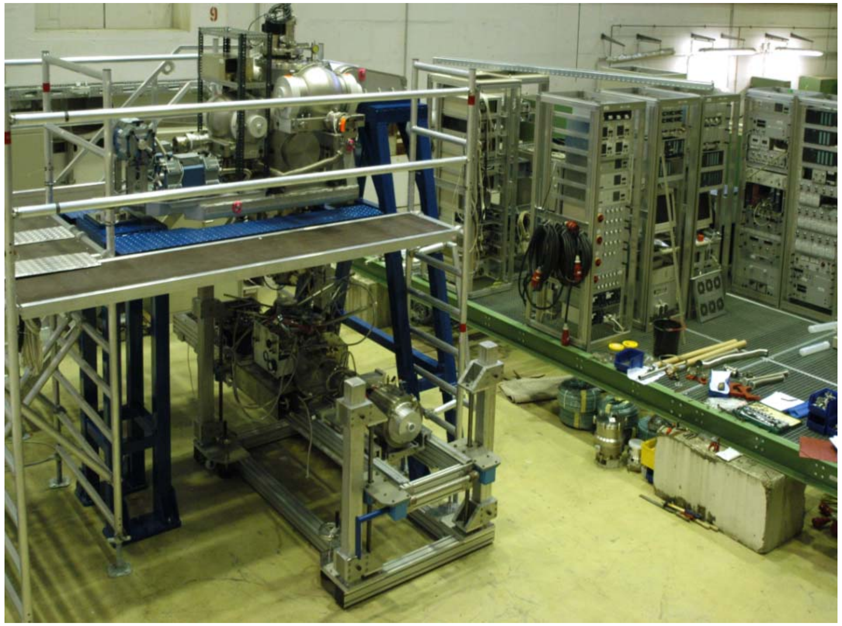
$$P = \frac{N_+ - N_-}{N_+ + N_-}$$

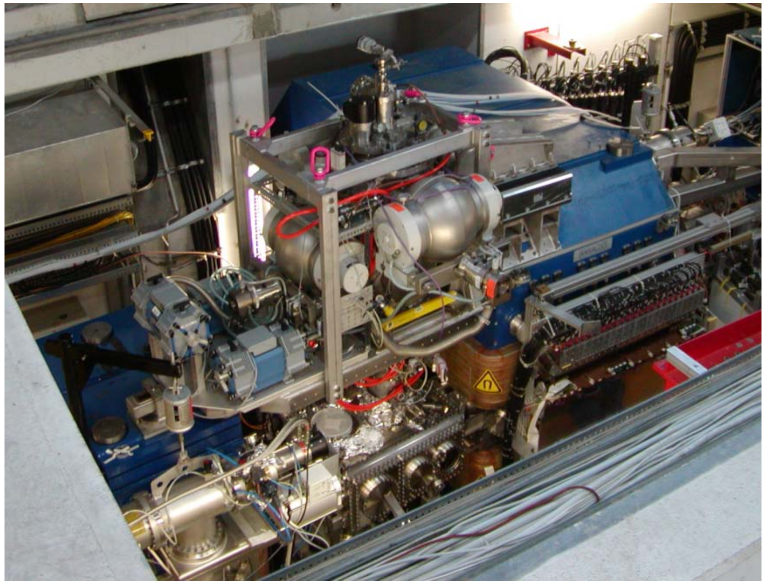


PIT @ ANKE/COSY

Main parts of a PIT:

- Atomic Beam Source
  - Target gas
    hydrogen or **deuterium**
  - H beam intensity (2 hyperfine states)
    $\mathbf{8.2 \cdot 10^{16}}$ **atoms / s**
  - Beam size at the interaction point
    $\boldsymbol{\sigma = 2.85 \pm 0.42}$ **mm**
  - Polarization for hydrogen atoms
    $\mathbf{P_Z = \ \ 0.89 \pm 0.01}$ **(HFS 1)**
    $\mathbf{P_Z = -0.96 \pm 0.01}$ **(HFS 3)**
- Lamb-Shift Polarimeter
- Storage Cell





M. Mikirtychyants et al.; NIM A **721** (0) 83 (2013)

Polarized H_2 Molecules

- Beam intensities of conventional ABS barely reach ~10^{17} at/s

$\Rightarrow$ target density d_t~10^{14} at/cm^2 (typical T-shaped storage cell)

- Depolarization at low T of storage cell don't allow further cooling

Performance of PIT using atomic beams saturates!

New storage cell materials

Polarized molecules?

Polarized H_2 Molecules

Measurements from NIKHEF, IUCF, HERMES show that recombined molecules retain fraction of initial nuclear polarization of atoms!

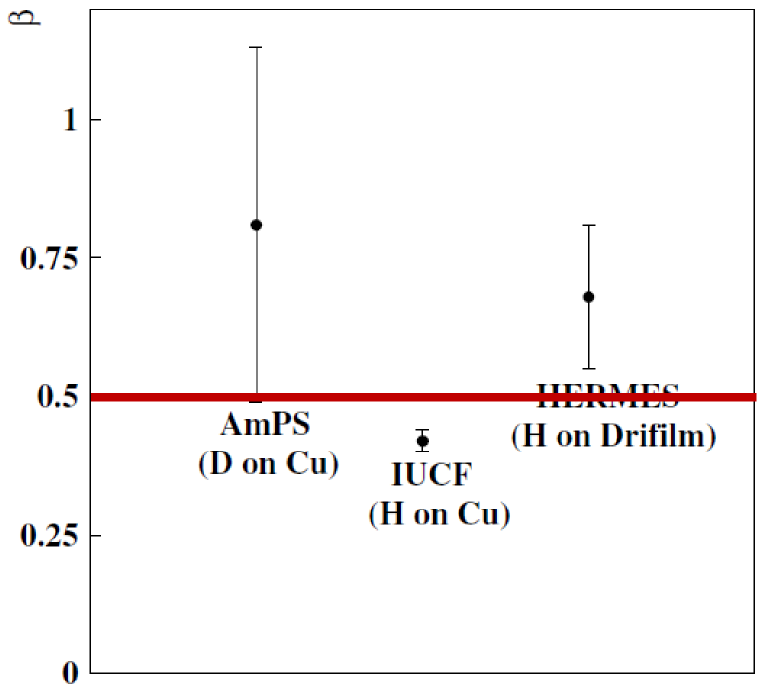


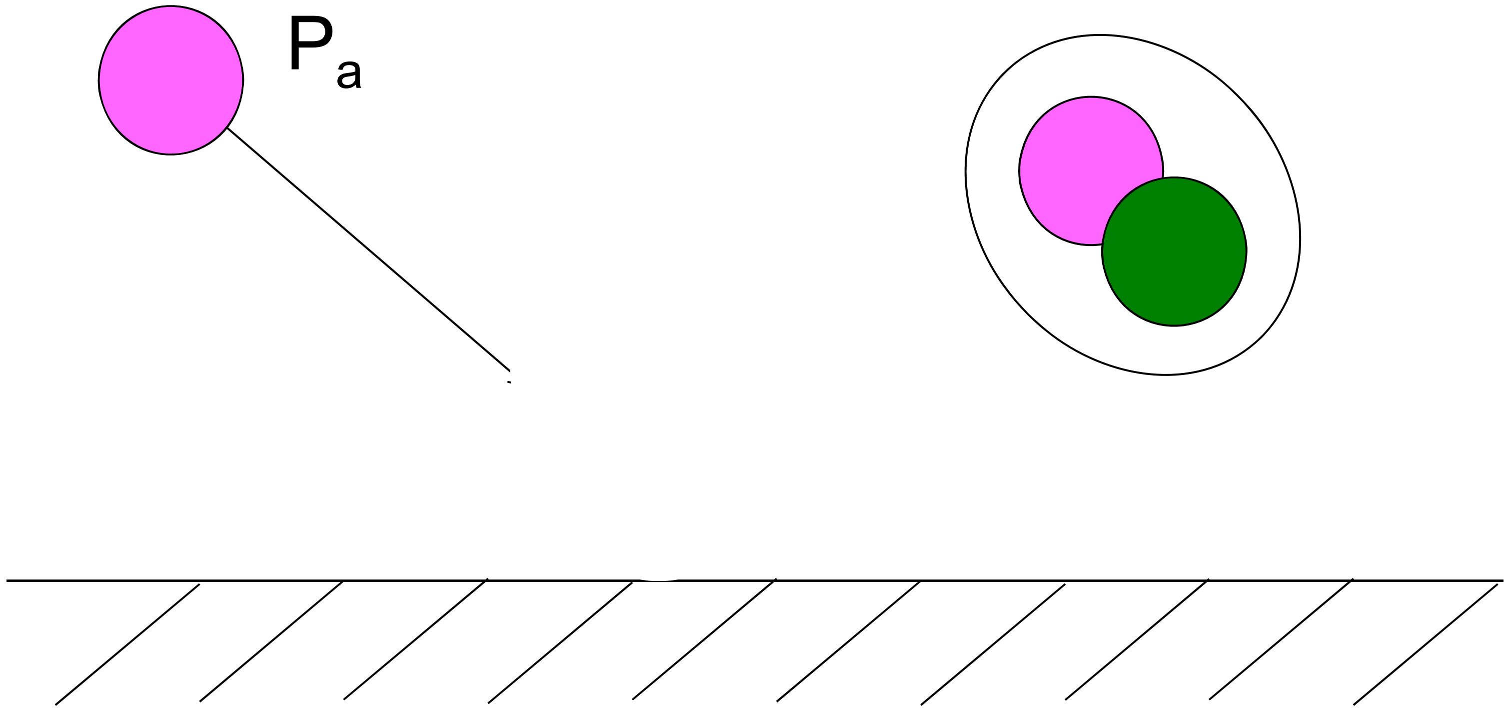
Fig. 2. Summary of the existing measurements of the nuclear polarization of recombined molecules. The newly obtained HERMES measurement at 260 K with a holding field of 330 mT is compared to the measurement by AmPS and IUCF obtained at room temperature and magnetic holding fields of 28 mT and 440 mT respectively.

The HERMES Collaboration; Eur. Phys. J. D **29**, 21–26 (2004)
DOI: 10.1140/epjd/e2004-00023-5

Polarized H_2 Molecules

Eley-Rideal Mechanism

$$P_m = 0.5\ P_a$$

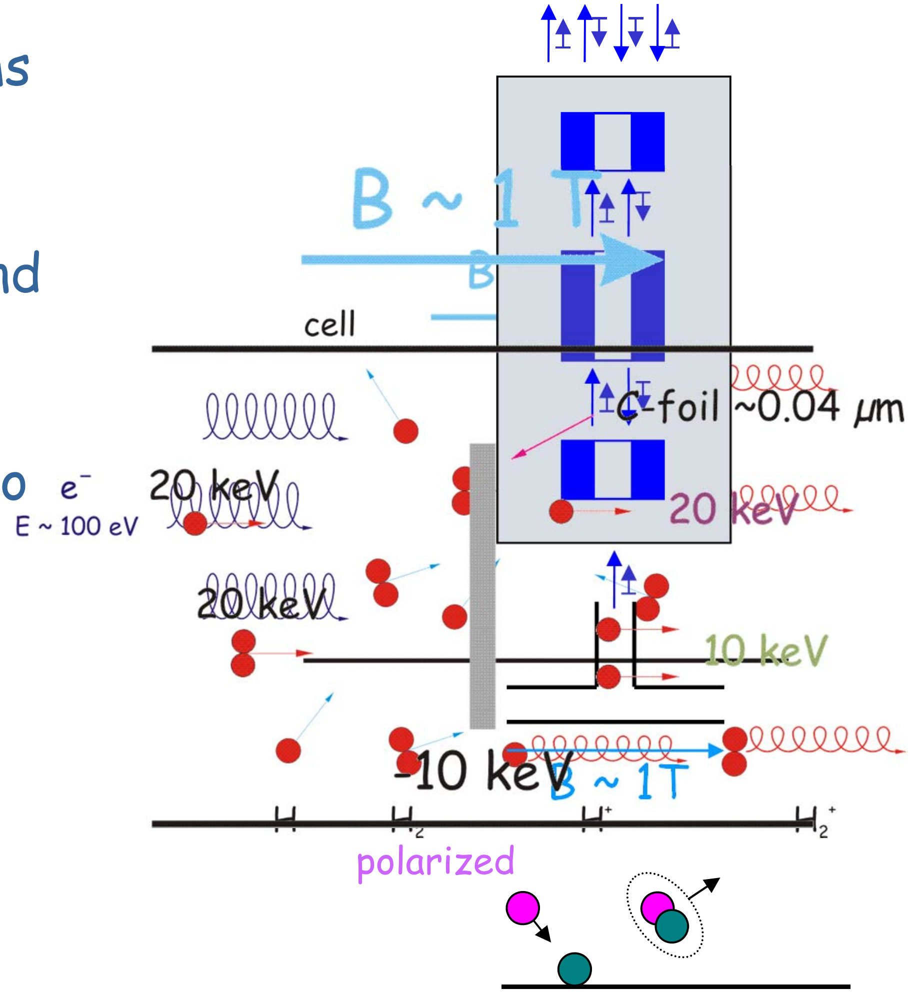


Is there a way to increase P_m

(surface material, T, B etc)?

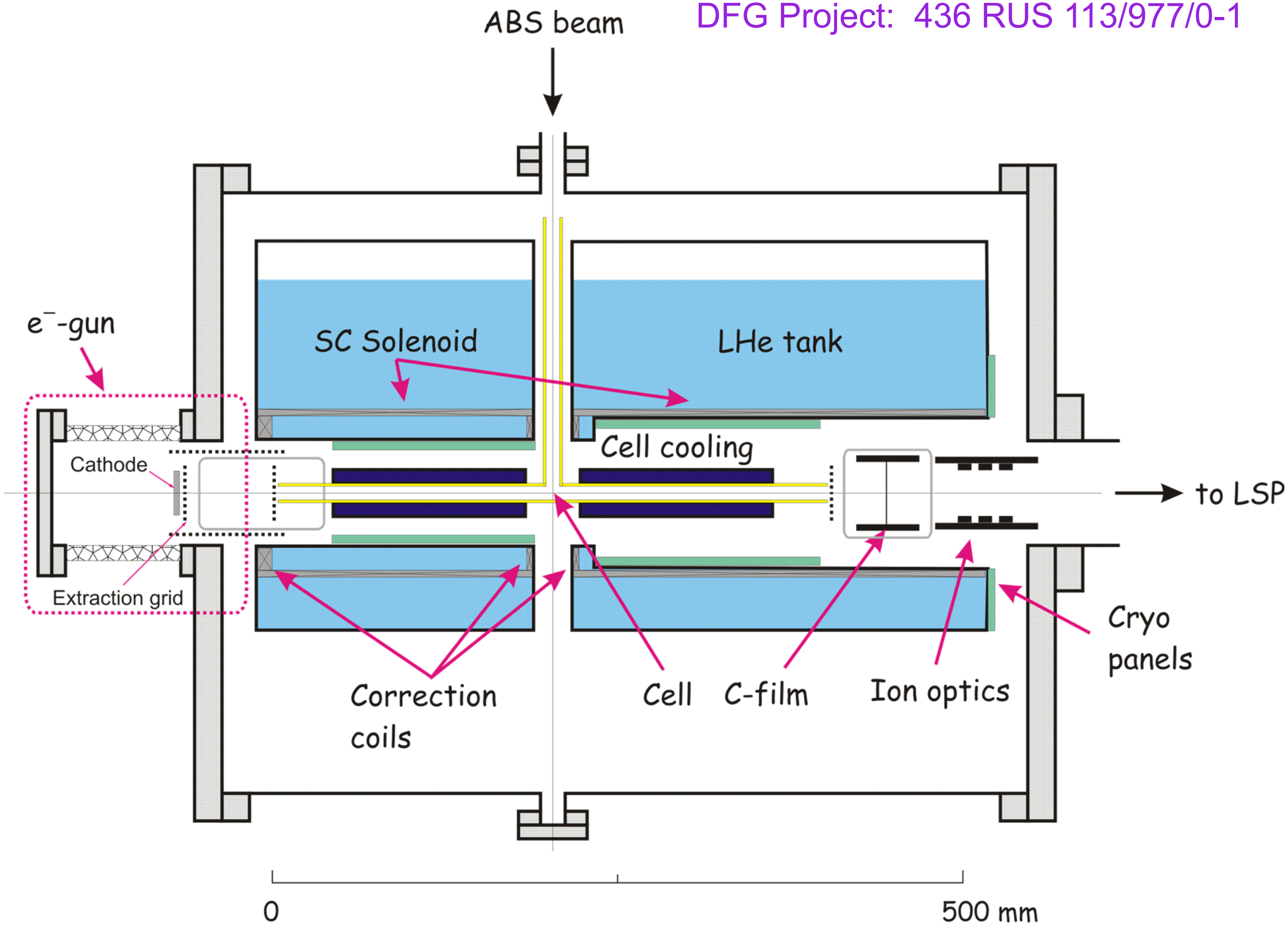
The original idea

- Recombination of polarized atoms into molecules
- Conversion of polarized atoms and molecules into ions
- Conversion of H_2^+ and H^+ ions into protons with different energy (suggested by W.Haeberli)
- Separation of protons by energy
- Measurement of proton polarization in LSP



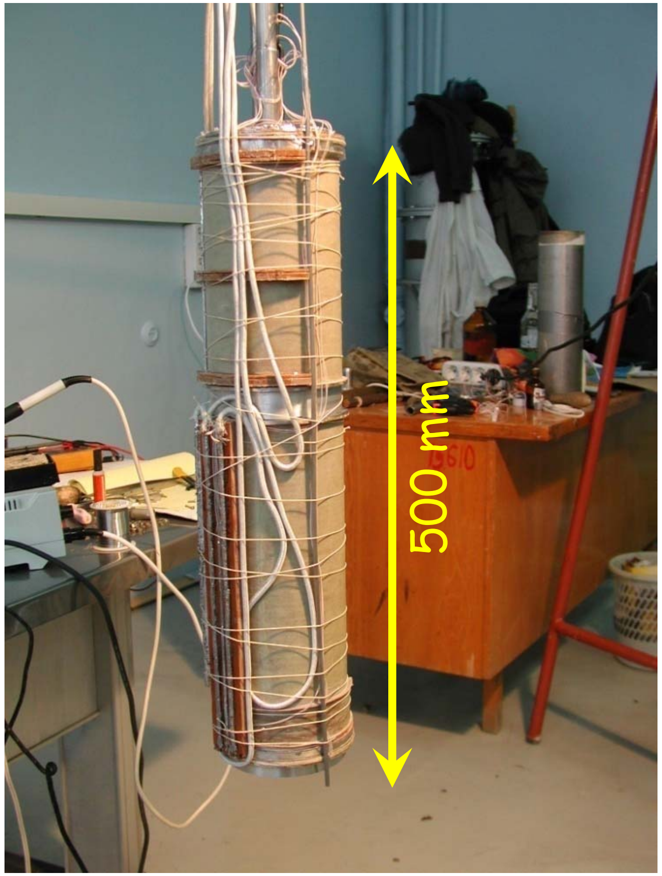
The experimental Setup

ISTC Project # 1861 PNPI, FZJ, Uni. Cologne
DFG Project: 436 RUS 113/977/0-1

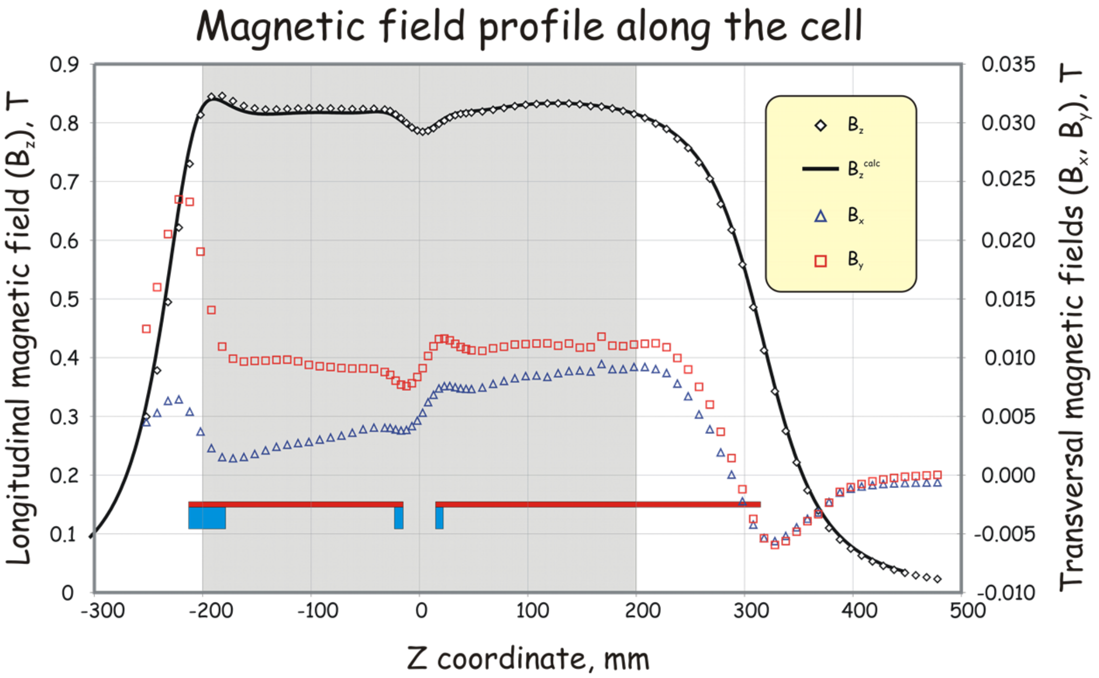


The experimental Setup

Superconducting Solenoid

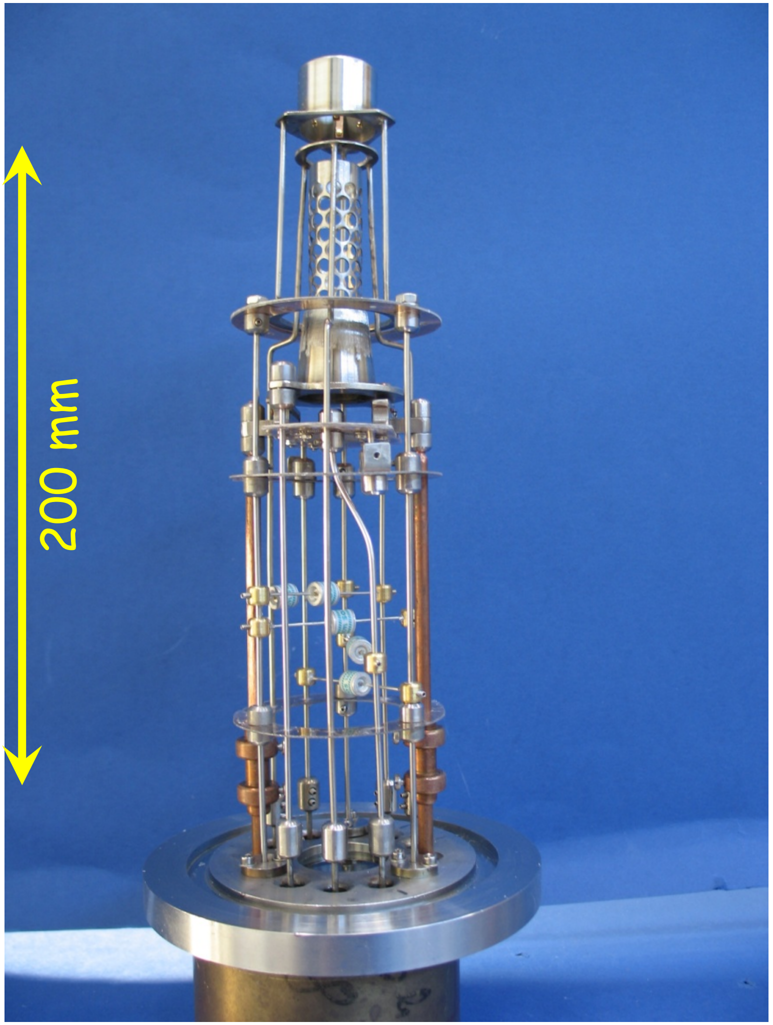


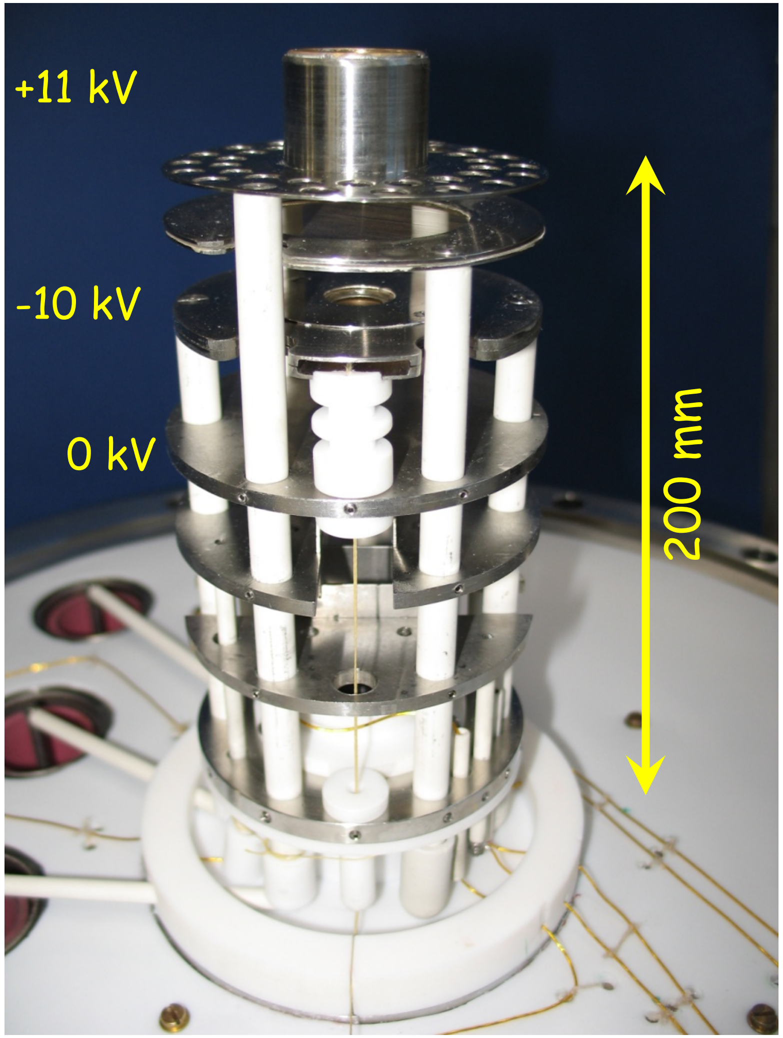
- SC wire NiTi+Cu (Ø 0.5 mm)
- Nominal current 50 A ⇒ B ~ 1 T
- Degradation of frozen field ≤ 0.1% per 5 hrs
- LHe consumption ~ 8 l/h



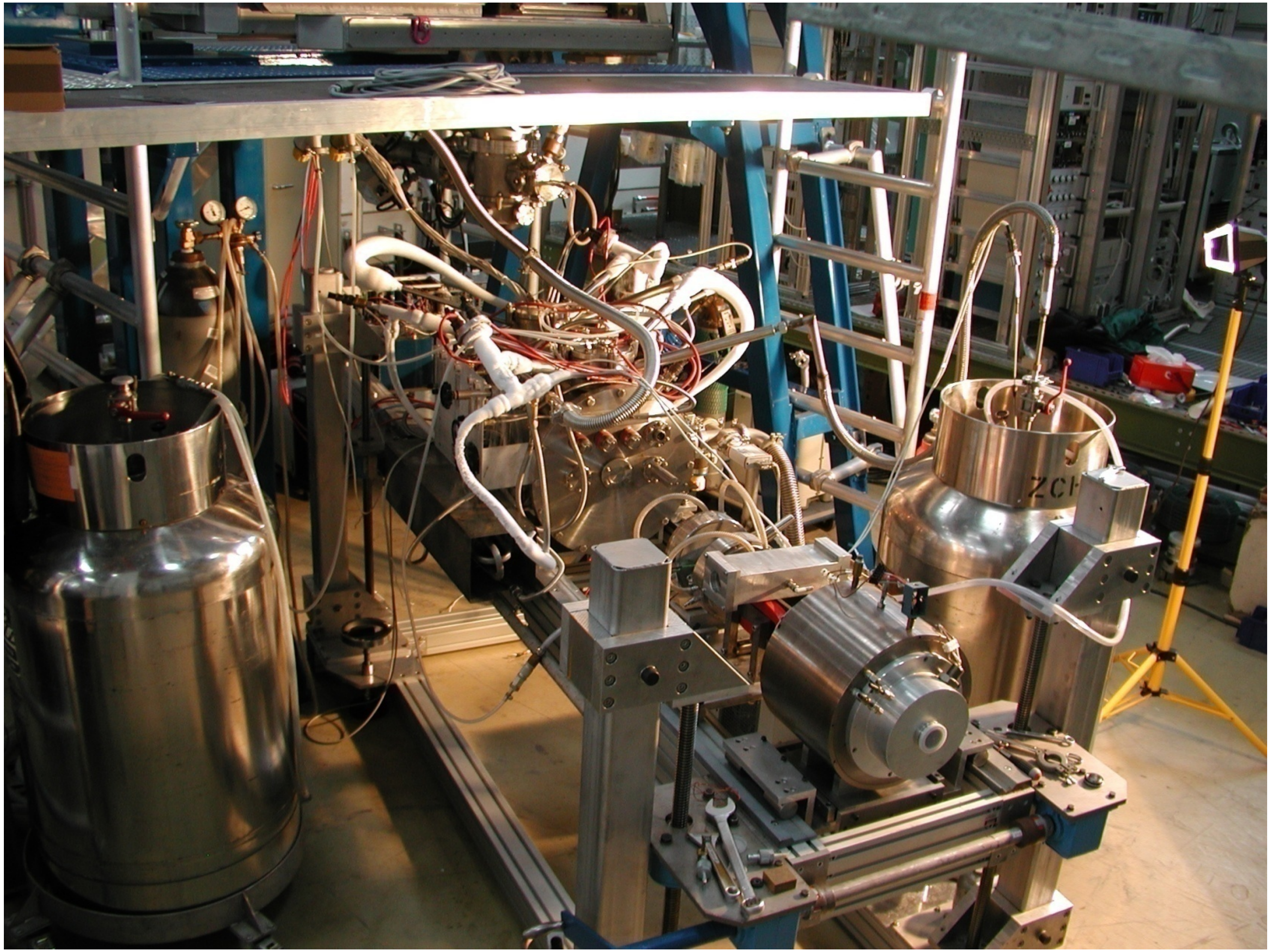
The experimental Setup

e⁻-gun and ion optics



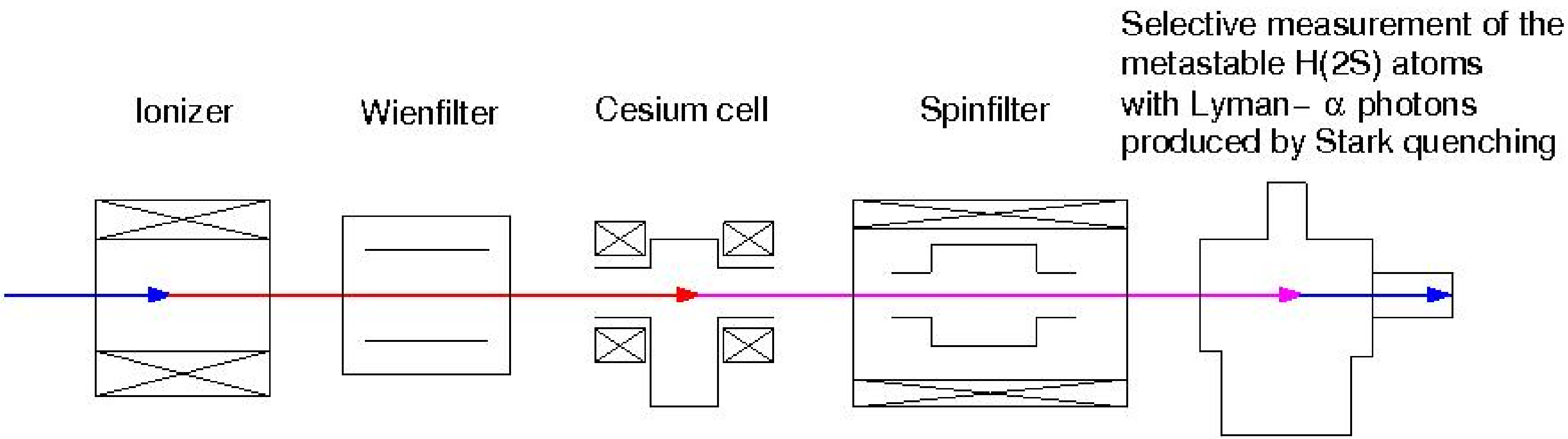


The experimental Setup



The experimental Setup

The Lamb-shift Polarimeter



$$\vec{H} \longrightarrow \vec{H}^{+} \longrightarrow \vec{H}^{+} \longrightarrow \vec{H}_{(2S)} \longrightarrow \vec{H}_{(2S_{m_I})} \longrightarrow H_{(1S)}$$

O^{+}
N^{+}

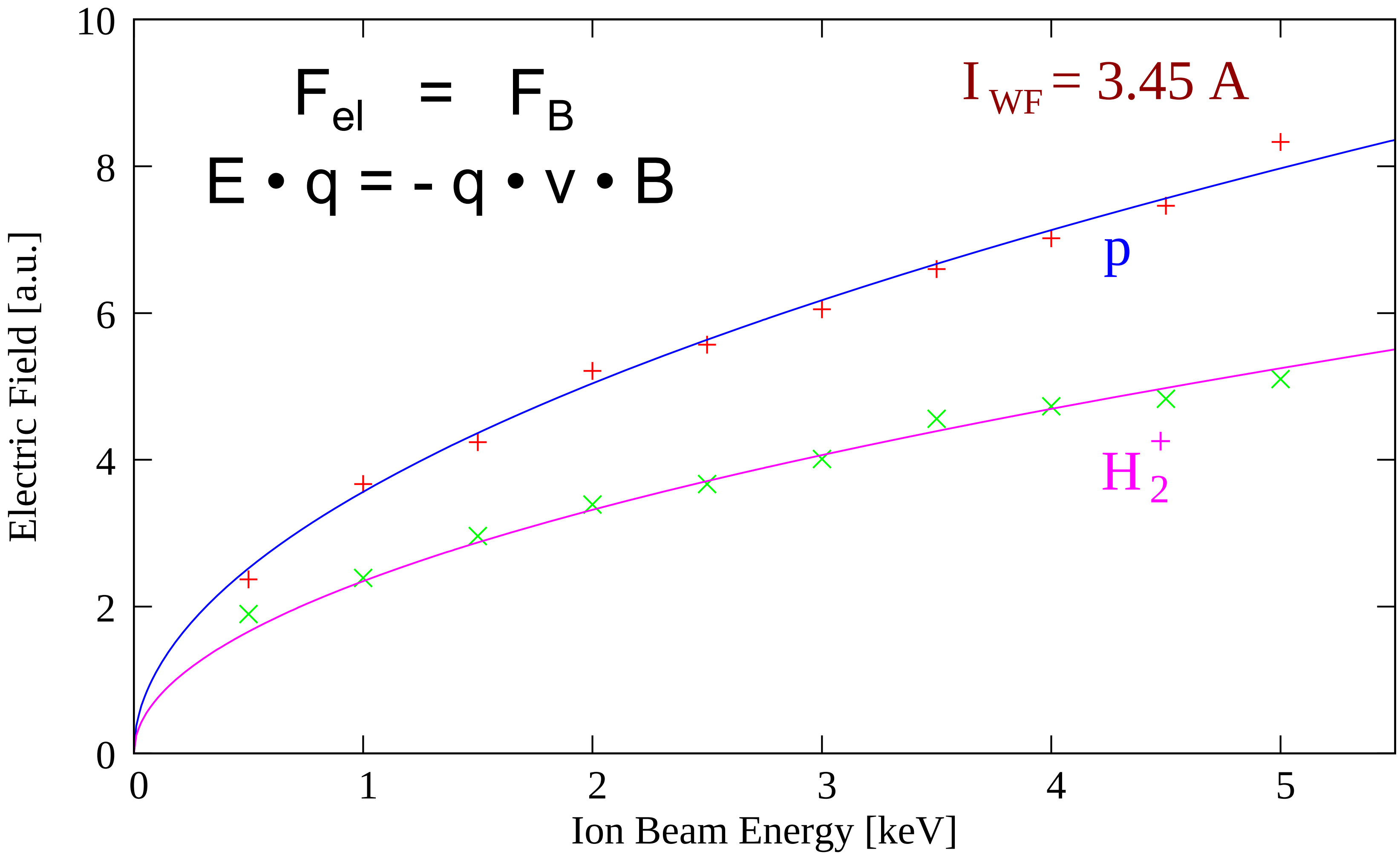
$\downarrow$ Ly_{α}

Efficiency: 10^{-10}

10^{-3} 10^{-1} 10^{-1} 10^{-3}

Experimental results

Mass separation with the Wienfilter

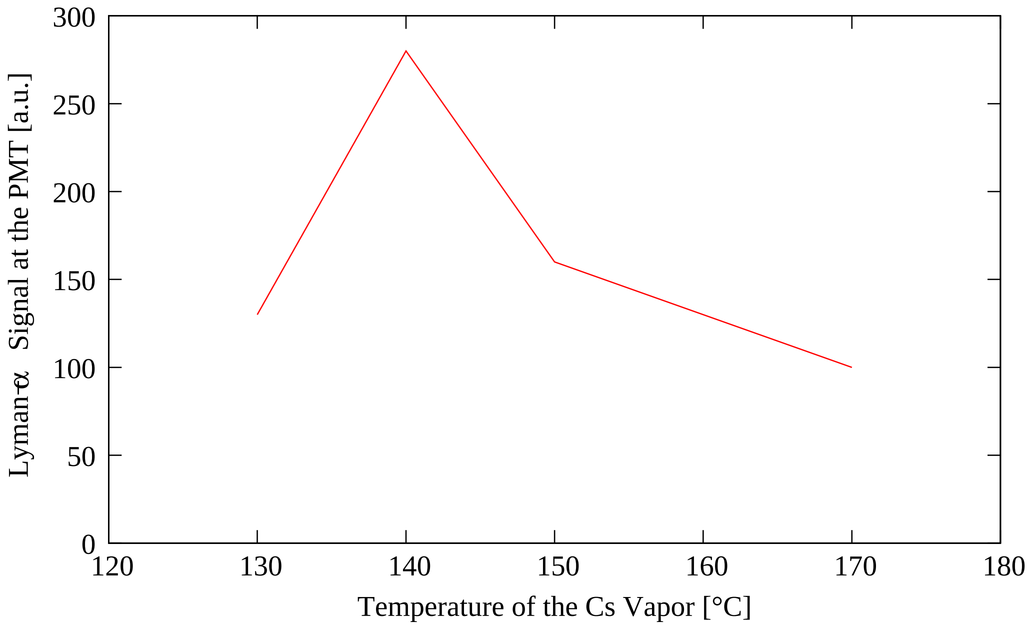


Experimental results

How are the polarized H_{2S} produced from H_2^+?

2-step process (Stripping at the Cs + H_{2S} production)

1-step process: Direct production: $H_2^+ + Cs \rightarrow H_{2S} + Cs^+ \ldots$



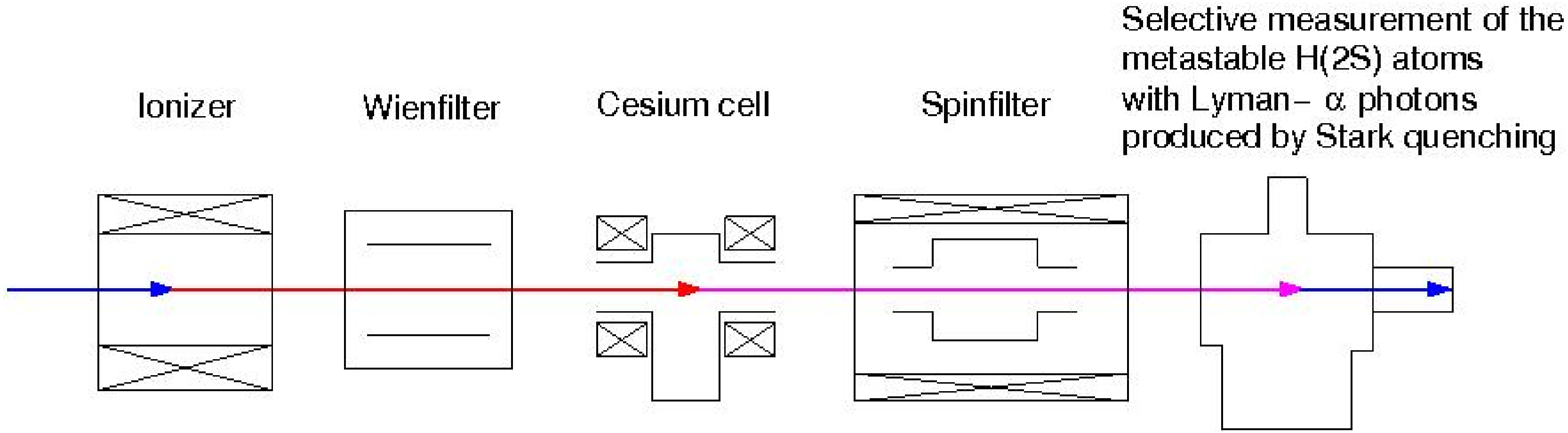
Cross section:

$\sigma(p \rightarrow H_{2S}) \approx 35 \cdot \sigma(H_2^+ \rightarrow H_{2S})$

R. Engels et al.;
Rev. Sci. Instr. **85** (2014)103505

The experimental Setup

The Lamb-shift Polarimeter



$$\vec{H} \longrightarrow \vec{H}^{+} \longrightarrow \vec{H}^{+} \longrightarrow \vec{H}_{(2S)} \longrightarrow \vec{H}_{(2S_{m_I})} \longrightarrow H_{(1S)}$$

O^{+}

N^{+}

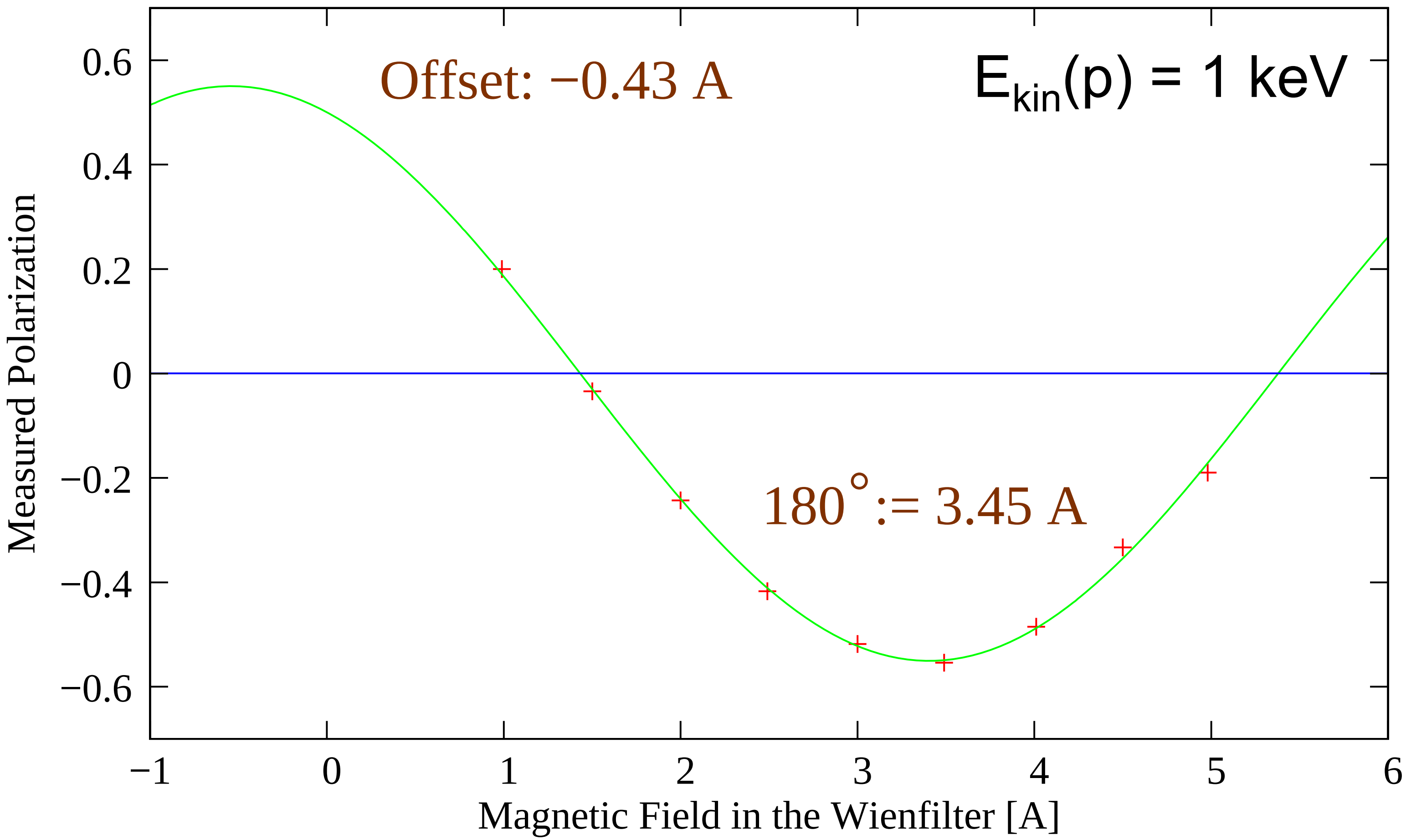
$\vec{H}_{(2S_{m_I})} \downarrow Ly_{\alpha}$

Efficiency: 10^{-10}

10^{-3} 10^{-1} 10^{-1} 10^{-3}

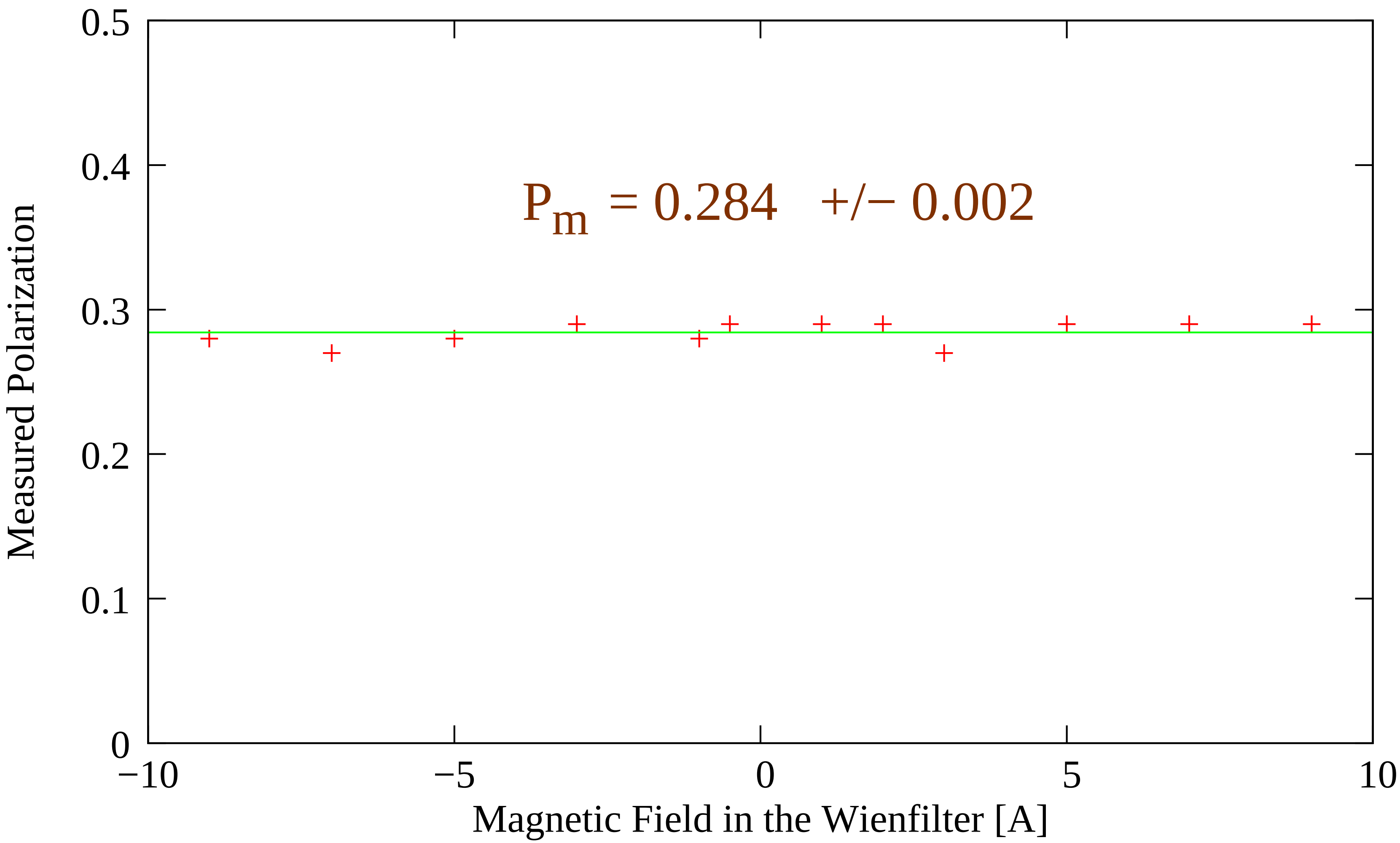
Experimental results

Wienfilter function of the protons in the LSP



Experimental results

Wienfilter function of the H_2^+ ions in the LSP



Important Details: H_2 Molecules

ortho-hydrogen	para-hydrogen
$\vert\uparrow\uparrow\rangle$	$\frac{1}{\sqrt{2}}(\vert\uparrow\downarrow\rangle - \vert\downarrow\uparrow\rangle)$
$\frac{1}{\sqrt{2}}(\vert\uparrow\downarrow\rangle + \vert\downarrow\uparrow\rangle)$	
$\vert\downarrow\downarrow\rangle$	

S=1 S=0

$o\text{-}H_2 \leftrightarrow p\text{-}H_2$: $\Delta E = -0.08$ kJ/mol

J = 1, 3, 5 J = 0, 2, 4

T= 300 K: 3 : 1

$T \rightarrow 0$ K: 0 : 4

Polarized H_2 Molecules

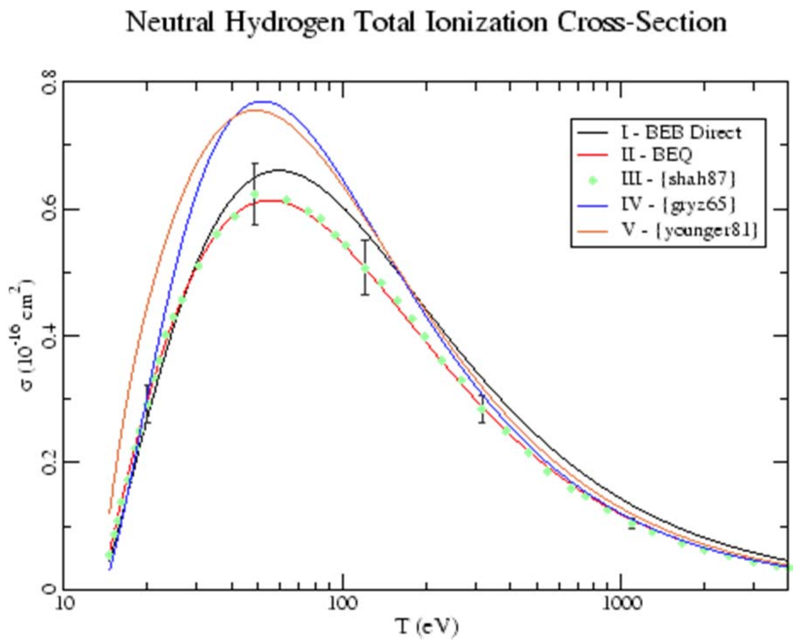
$\Psi_{a,b}(I, m_I)$ and $I_a = 1,\ I_b = 1$
ortho-deuterium
$\Psi(2,2) = \Psi_a(1,1)\Psi_b(1,1)$
$\Psi(2,1) = \frac{1}{\sqrt{2}}[\Psi_a(1,0)\Psi_b(1,1) + \Psi_a(1,1)\Psi_b(1,0)]$
$\Psi(2,0) = \frac{1}{\sqrt{6}}[\Psi_a(1,1)\Psi_b(1,-1) + 2\Psi_a(1,0)\Psi_b(1,0) + \Psi_a(1,-1)\Psi_b(1,1)]$
$\Psi(2,\text{-}1) = \frac{1}{\sqrt{2}}[\Psi_a(1,0)\Psi_b(1,-1) + \Psi_a(1,-1)\Psi_b(1,0)]$
$\Psi(2,-2) = \Psi_a(1,-1)\Psi_b(1,-1)$
$\Psi(0,0) = \frac{1}{\sqrt{3}}[\Psi_a(1,1)\Psi_b(1,-1) - \Psi_a(1,0)\Psi_b(1,0) + \Psi_a(1,-1)\Psi_b(1,1)]$
para-deuterium
$\Psi(1,1) = \frac{1}{\sqrt{2}}[\Psi_a(1,1)\Psi_b(1,0) - \Psi_a(1,0)\Psi_b(1,1)]$
$\Psi(1,0) = \frac{1}{\sqrt{2}}[\Psi_a(1,+1)\Psi_b(1,-1) - \Psi_a(1,-1)\Psi_b(1,1)]$
$\Psi(1,-1) = \frac{1}{\sqrt{2}}[\Psi_a(1,0)\Psi_b(1,-1) - \Psi_a(1,-1)\Psi_b(1,0)]$

S=0 and S=2 are the groundstates

The Ionization Processes

$$H + e \rightarrow H^{+} + 2e$$

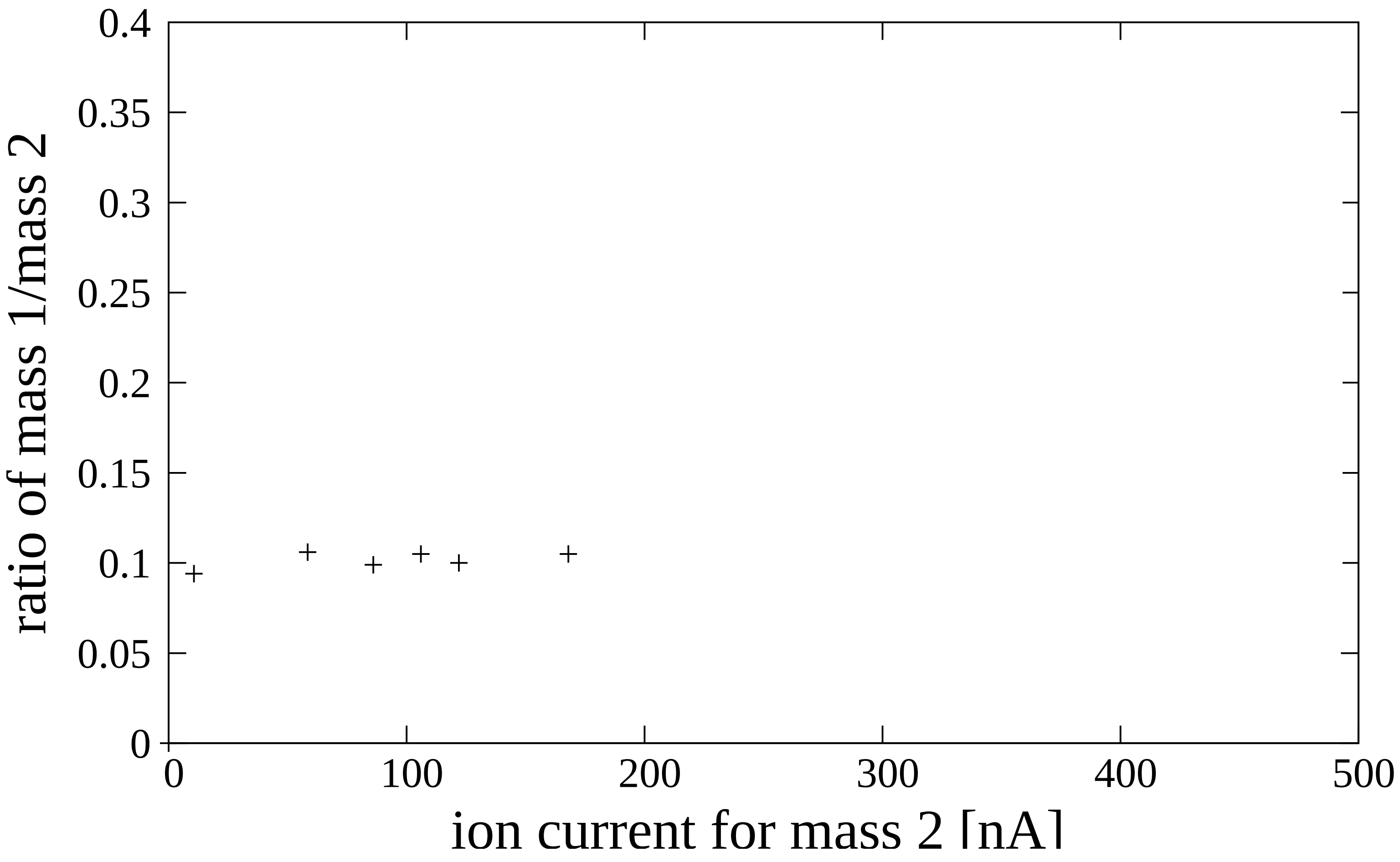
(E_e = 150 eV: $\sigma = 0.46 \cdot 10^{-16}$ cm^2)



(www.nist.gov)

Recombination

Storage cell filled with H_2 gas with different fluxes



Polarized H_2 Molecules

Polarization losses of the molecules

A. Abragam: The Principles of Nuclear Magnetism (1961)

Spin Relaxation of H_2/D_2 Molecules

→ The polarization losses during wall collision depend on:

- Nuclear Spin I
- Polarization P_m
- Temperature
- Magnetic field in the cell

Theory

A. Abragam: The Principles of Nuclear Magnetism

Hamiltonian to describe the nuclear relaxation of a H_2 molecules

$$\boxed{H = \omega_I \left(I^1_z + I^2_z \right) + \omega_J J_z + \omega' \left(\mathbf{I^1} + \mathbf{I^2}\right)\cdot\mathbf{J} + \omega'' \left\{ \mathbf{I^1}\cdot \mathbf{I^2} - 3(\mathbf{I^1}\cdot \mathbf{n})(\mathbf{I^2}\cdot \mathbf{n})\right\}}$$

$\mathbf{I^1}$ and $\mathbf{I^2}$ are the spins of the two protons

$\mathbf{I^1} + \mathbf{I^2} = \mathbf{I}$

$\mathbf{J}$ is the rotational angular momentum of the molecule

$\omega_I = -\gamma_I H_0$ is the proton Lamor frequency in the applied field H_0

$\omega_J = -\gamma_J H_0$ is the Lamor frequency of the rotational magnetic moment of the H_2

$\omega' = -\gamma_I H'$ is the strength of the coupling between the magnetic moment of the protons and the magnetic field produced at their positions by the rotation of the molecule ($H' = 2.7$ mT)

$\omega'' = 2\gamma_I H'' = \gamma_I^2 \hbar / b^3$ is the strength of the dipolar coupling between the protons, b is their distance, and $\mathbf{n}$ is the unit vector $\mathbf{b}/b$ ($H'' = 3.4$ mT).

Polarized H_2 Molecules

Polarization losses of the molecules

A. Abragam: The Principles of Nuclear Magnetism (1961)

Spin Relaxation of H_2/D_2 Molecules

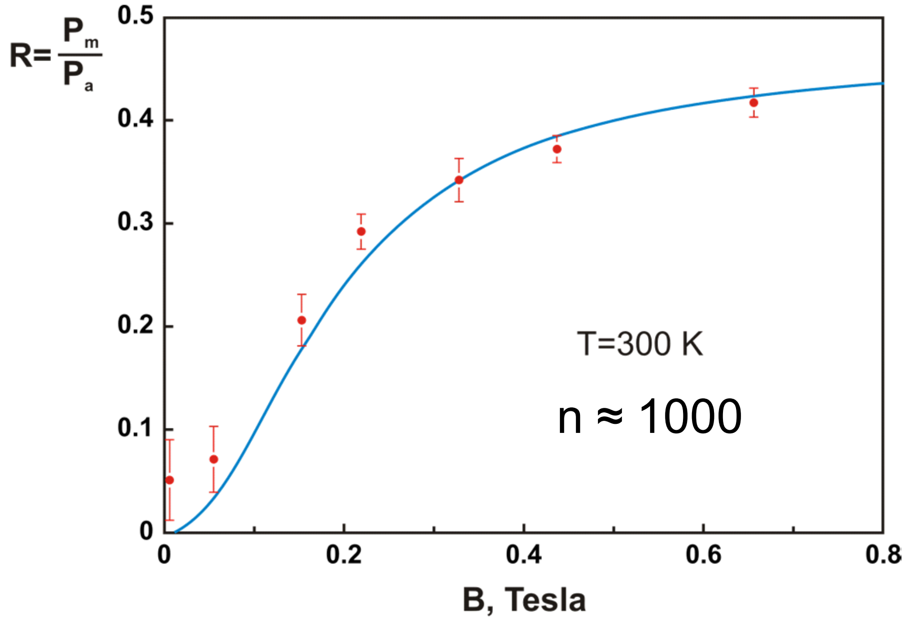
→ The polarization losses during wall collision depend on:

- Nuclear Spin I
- Polarization P_m
- Temperature
- Magnetic field in the cell

$$P_{(B,n)} = P_m \cdot e^{-n\left(\frac{B_c}{B}\right)^2}$$

$\Rightarrow$ $B_c = 5.4$ mT

(For T ~ 100 K)

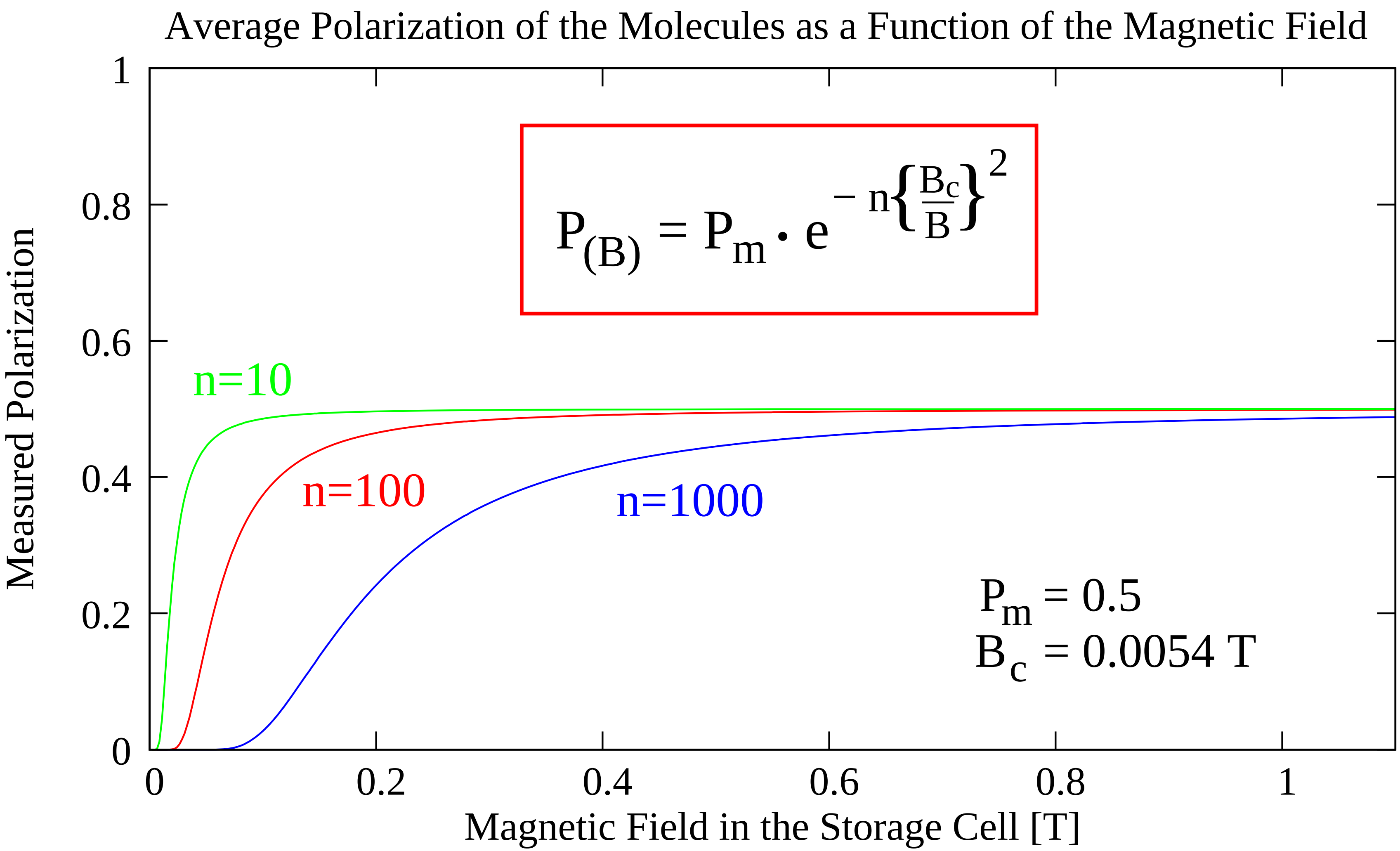


Nuclear Polarization of Hydrogen Molecules from Recombination of Polarized Atoms

T.Wise et al., Phys. Rev. Lett. 87, 042701 (2001).

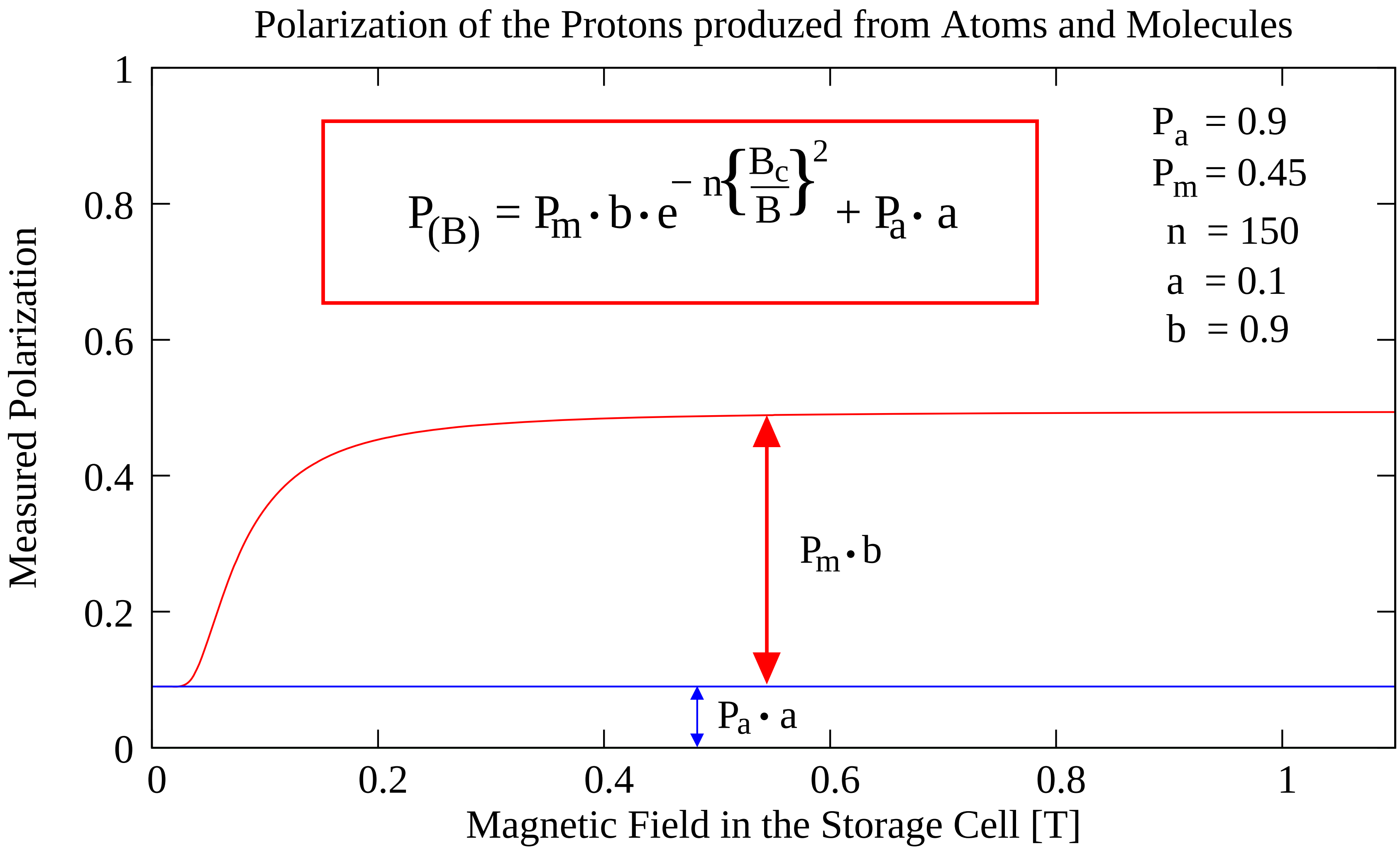
$$\lim_{B\to\infty} R = 0.5$$

Theory

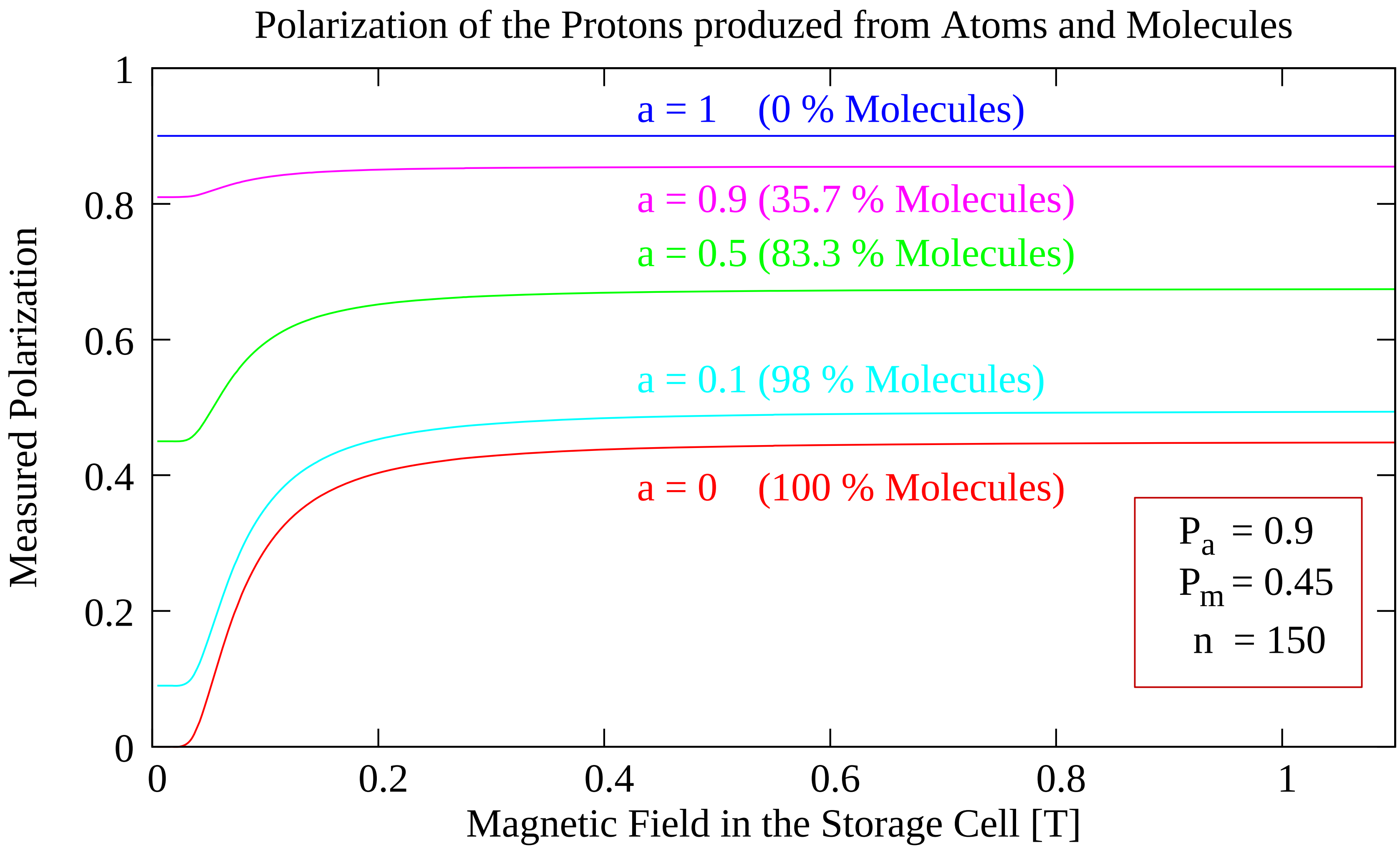


Average Polarization of the Molecules as a Function of the Magnetic Field
$P_{(B)} = P_m \cdot e^{-n\left\{\frac{B_c}{B}\right\}^2}$
n=10
n=100
n=1000
$P_m = 0.5$
$B_c = 0.0054$ T
Measured Polarization
Magnetic Field in the Storage Cell [T]
0
0.2
0.4
0.6
0.8
1

Theory

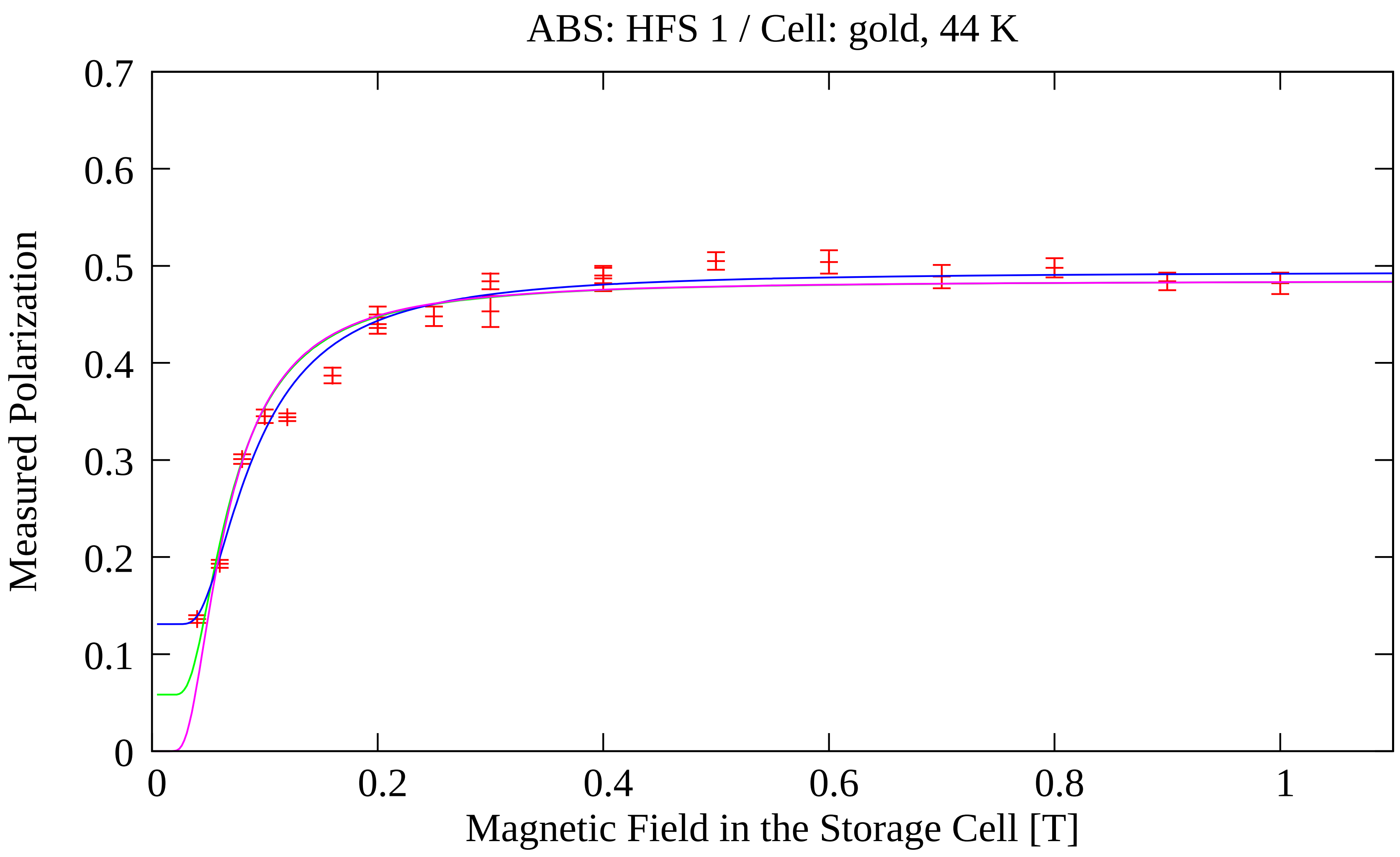

Polarization of the Protons produzed from Atoms and Molecules
$P_{(B)} = P_m \cdot b \cdot e^{-n\left\{\frac{B_c}{B}\right\}^2} + P_a \cdot a$
$P_a = 0.9$
$P_m = 0.45$
$n = 150$
$a = 0.1$
$b = 0.9$
$P_m \cdot b$
$P_a \cdot a$
Measured Polarization
Magnetic Field in the Storage Cell [T]
0
0.2
0.4
0.6
0.8
1

Theory



Polarization of the Protons produzed from Atoms and Molecules
a = 1 (0 % Molecules)
a = 0.9 (35.7 % Molecules)
a = 0.5 (83.3 % Molecules)
a = 0.1 (98 % Molecules)
a = 0 (100 % Molecules)
P_a = 0.9
P_m = 0.45
n = 150
Measured Polarization
0
0.2
0.4
0.6
0.8
1
0
0.2
0.4
0.6
0.8
1
Magnetic Field in the Storage Cell [T]

Experimental results: Polarization of Protons



n can have different distributions W(n) !

Simpelst Case (zylindrical geometries / elastic scattering):

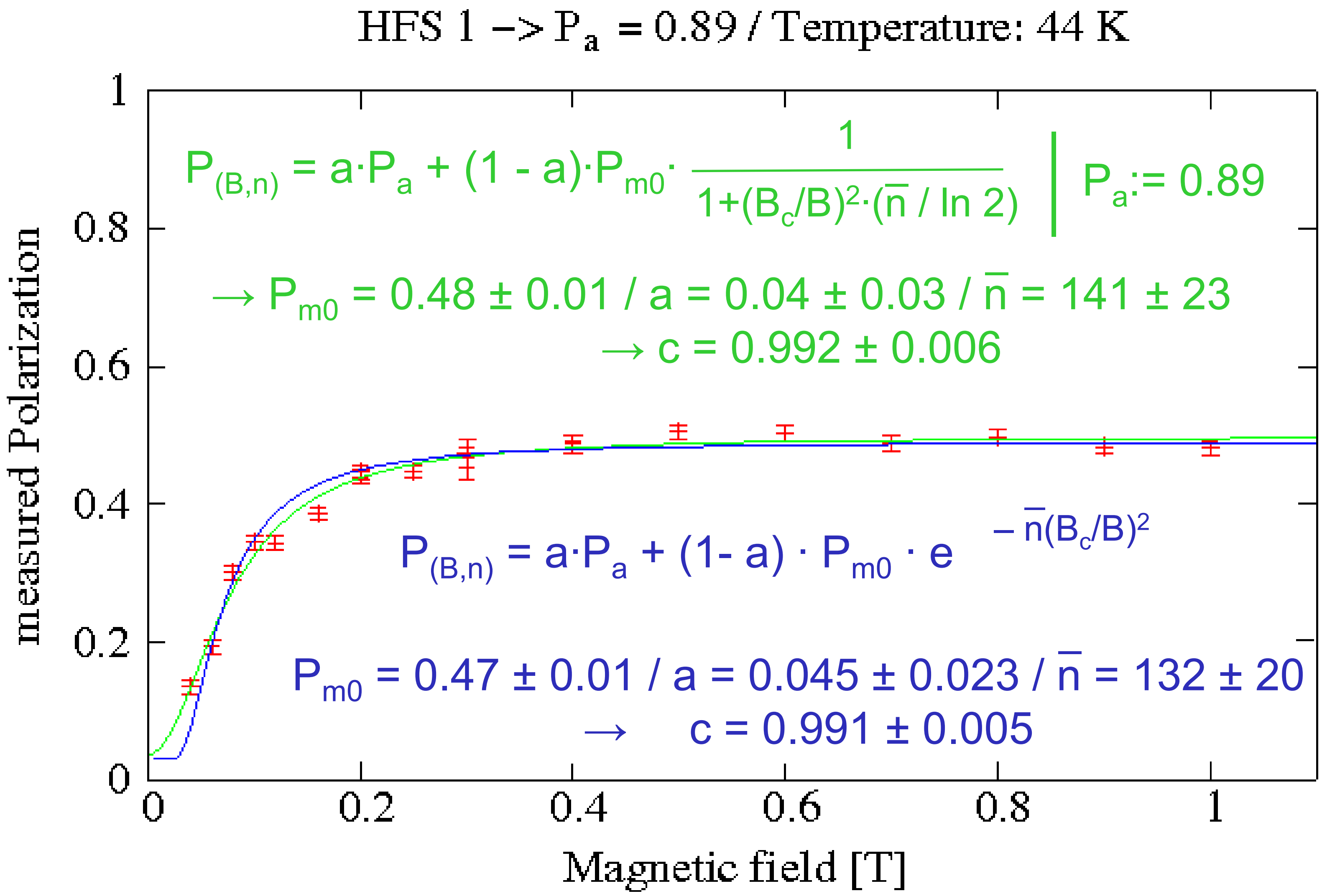
$$\rightarrow \qquad W_{(n)} = 1/\alpha \;\; e^{-\alpha n}$$

$$\rightarrow \qquad \bar{n} = \ln 2 / \alpha$$

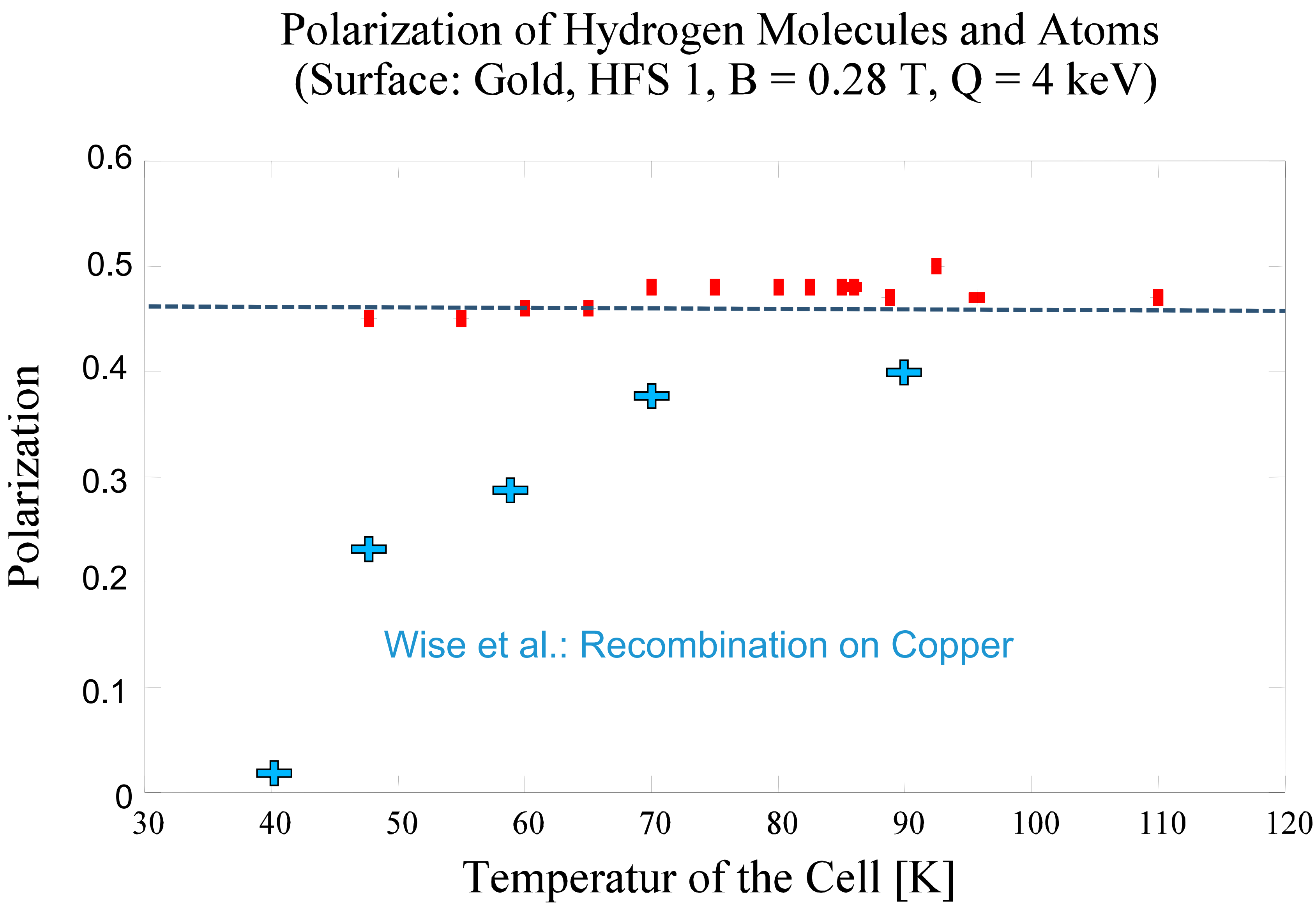
$$\rightarrow \qquad P_m(B,n) = P_{m_0} \cdot \frac{1}{1+(B_c/B)^2 \cdot \bar{n}/\ln 2}$$

More complicated cases (e.g. $\cos^{0,1,2,\dots}$ distribution of the molecules, when they are leaving the surface) deliver different W(n) and $\bar{n}$.

Experimental results: Polarization of Protons



Experimental results



Experimental results

J.S. Price and W. Haeberli,

"Measurement of cell wall depolarization of polarized hydrogen gas targets in a weak magnetic field"

Nuclear Instruments and Methods in Physics Research A **349** (1994) 321-333

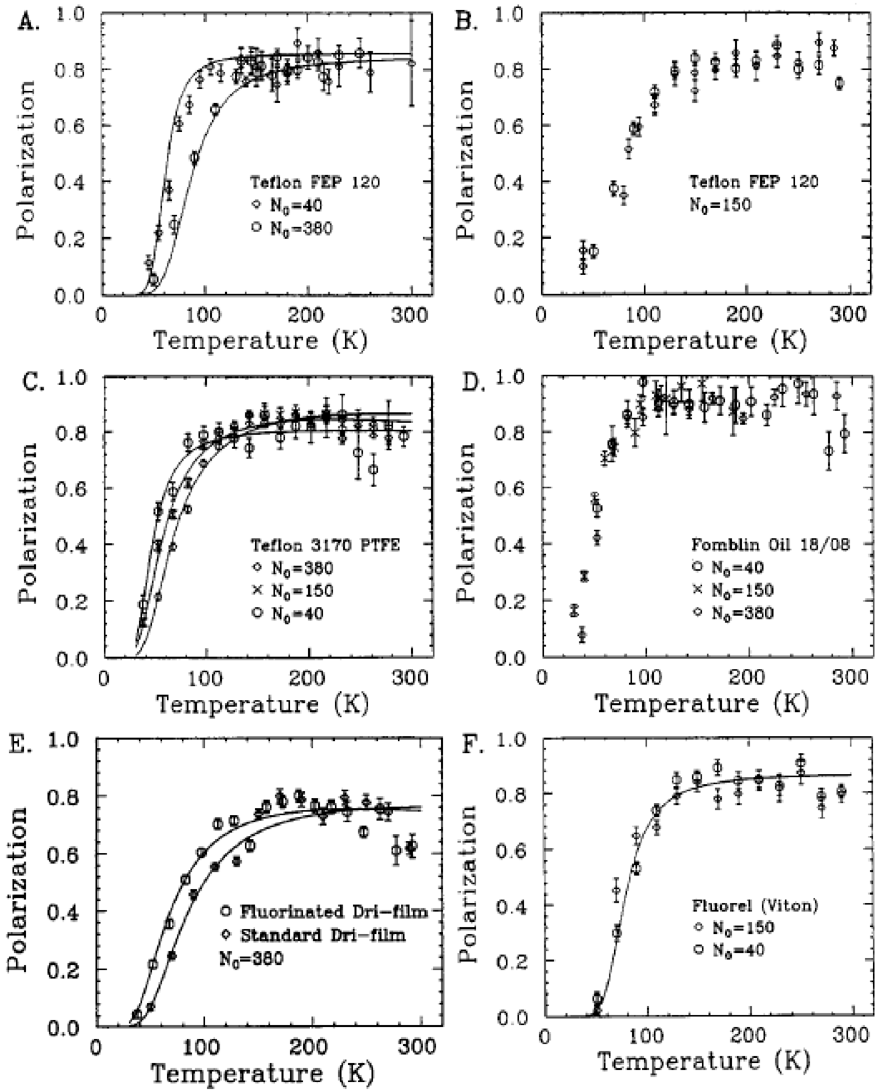


Fig. 4. Measured $\vec{H}^0$ target polarization vs. cell wall temperature for Teflon, Fomblin, Dri-film and Viton coated onto 6061 aluminum cells. Polarization is expressed as a fraction of the expected maximum assuming no depolarization. N_0 is the average age of the target atoms in number of wall collisions. The solid lines are curves fit to the data as described in Section 7.

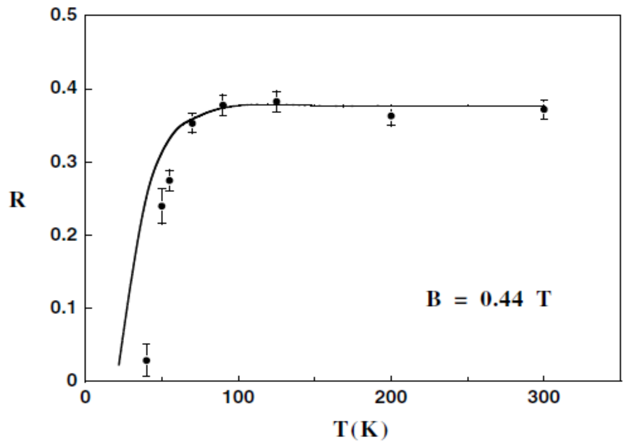
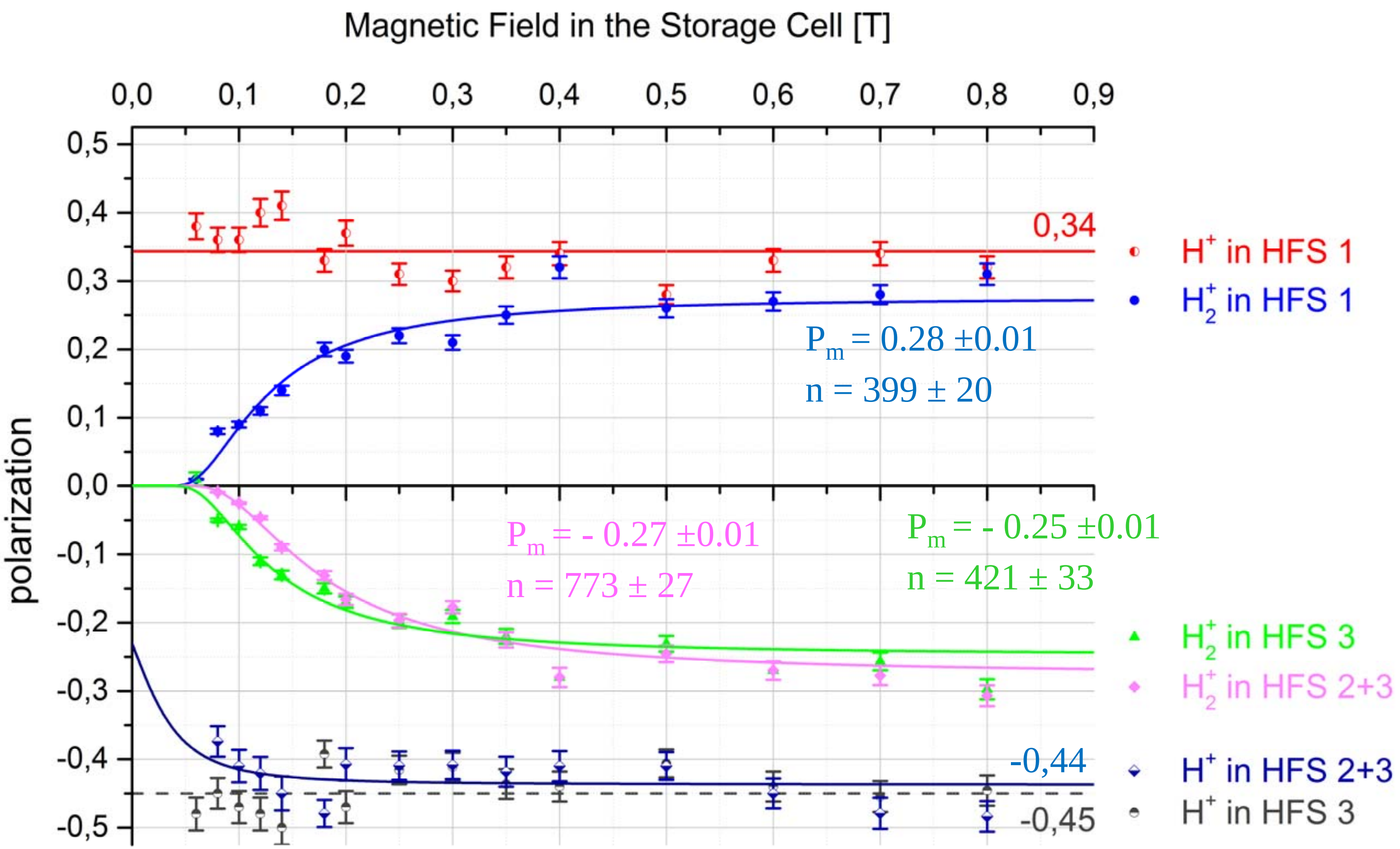


FIG. 3. Fraction R of proton polarization of the H atoms that is retained in the H_2 molecules after recombination on a copper surface at different temperatures T for a fixed magnetic field strength $B = 0.44$ T. The curve is based on measurements of the polarization of hydrogen *atoms* in a Cu cell in which about 65% of the atoms recombined; see Ref. [15].

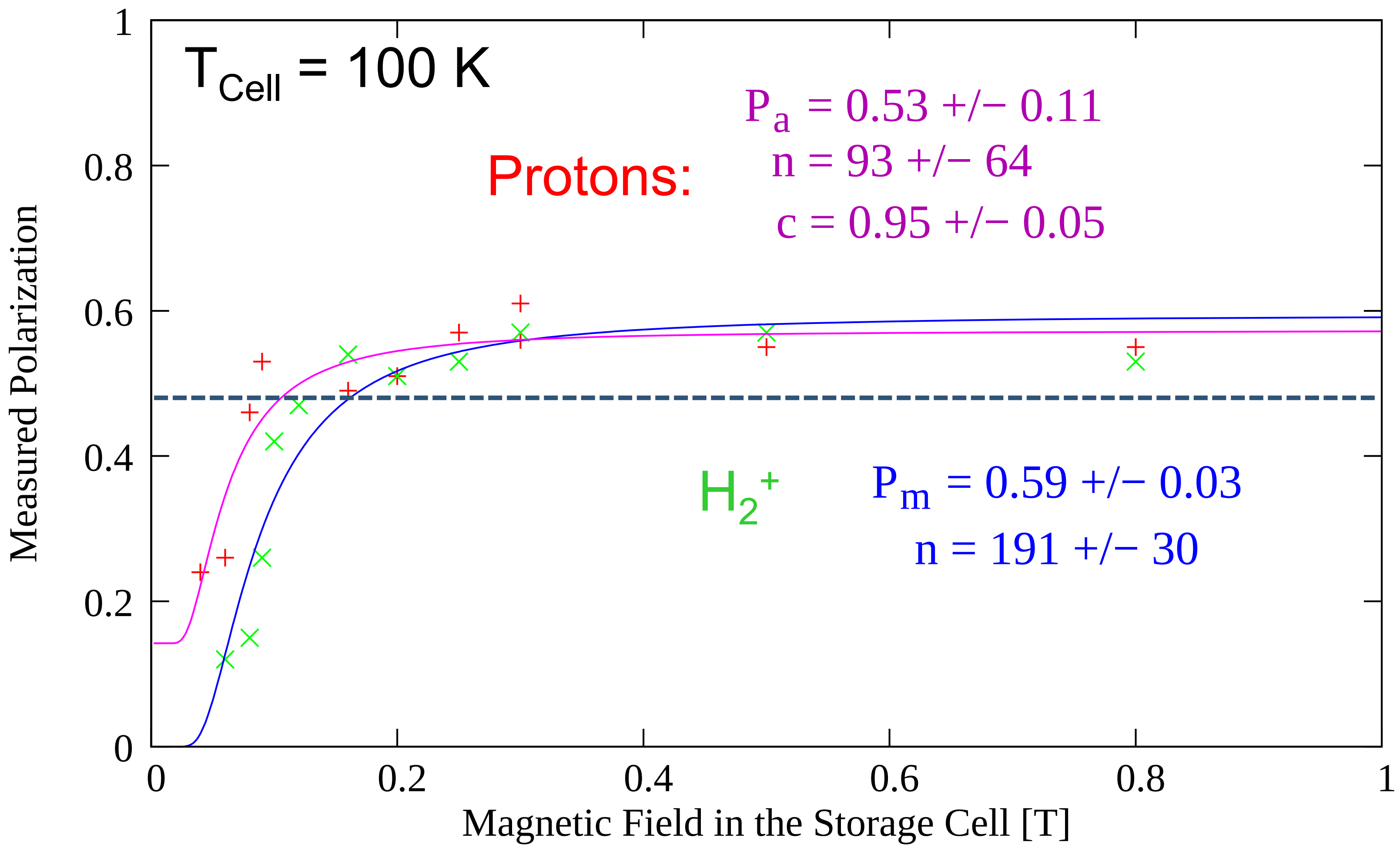
Experimental results

Very first results on water: T_{cell} = 100 K (on fuzed quarz)



Experimental results

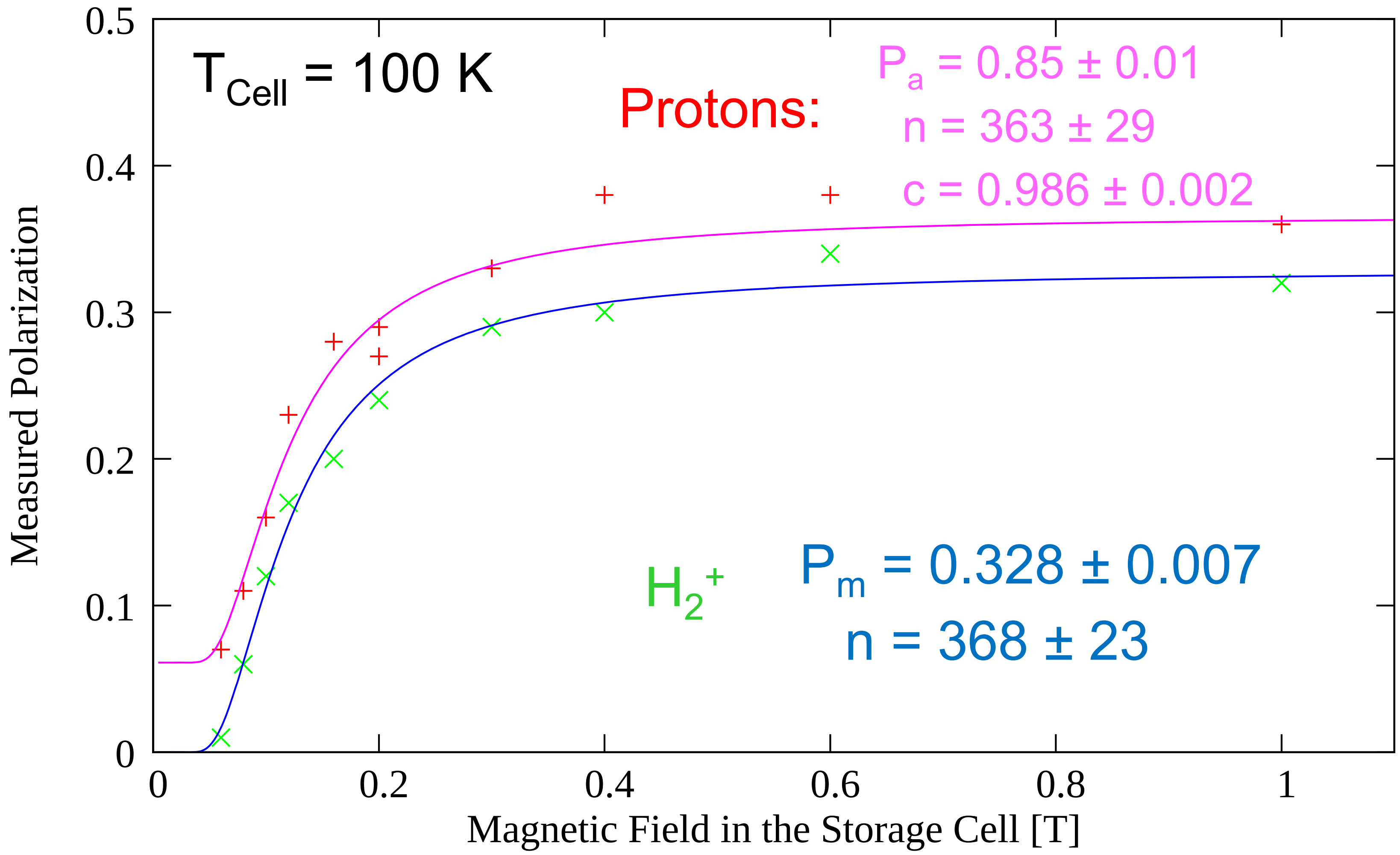
Measurements on Fused Quartz Glass in the first hours



P_m = 66 % of the original atomic Polarization

Experimental results

Measurements on Fused Quartz Glass after several days

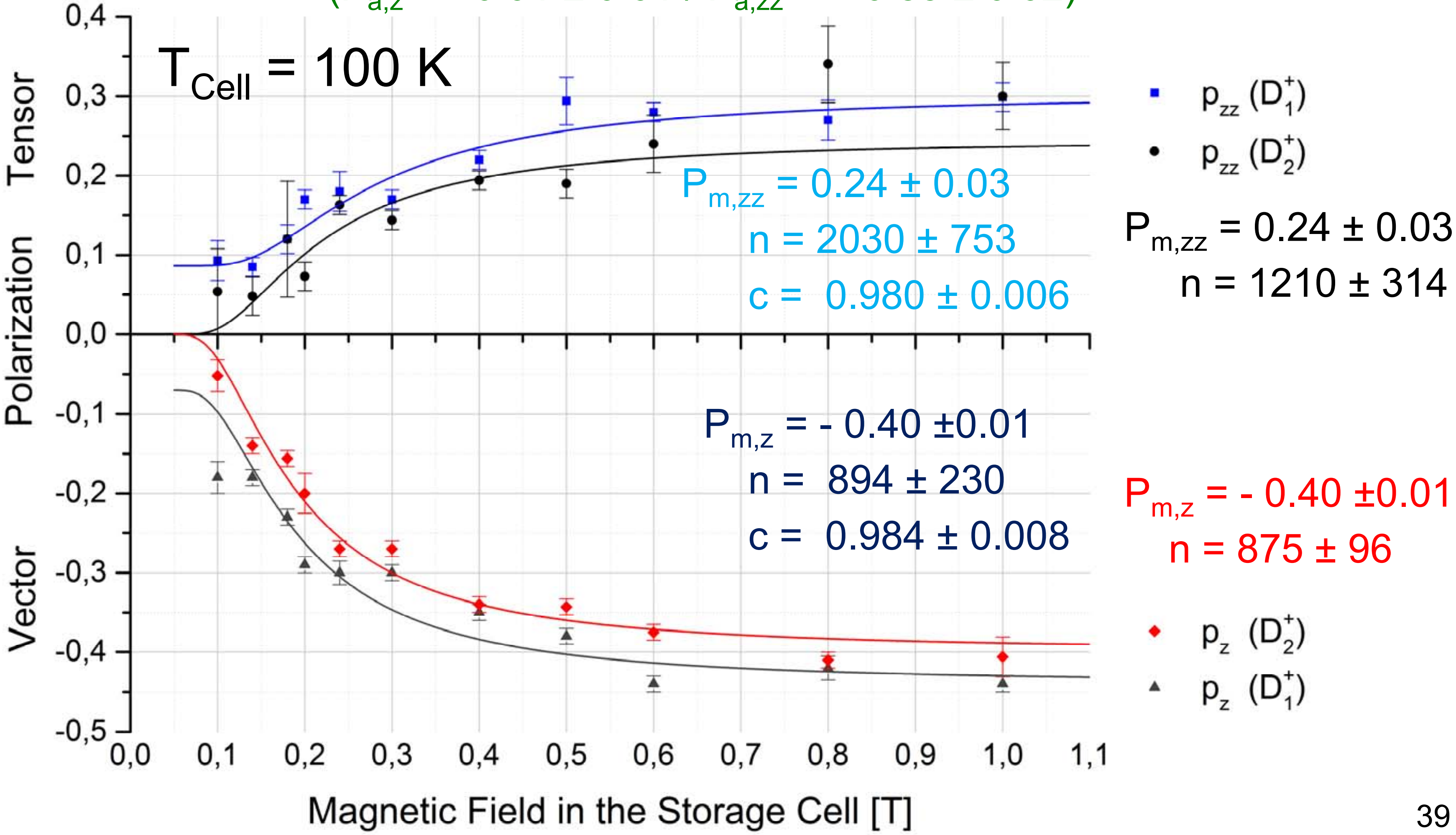


Experimental results

Measurements on Fused Quartz Glass after several days

Deuterium: HFS 3+4 (Vector and Tensorpolarized)

($P_{a,z}$ = - 0.91 ± 0.01 / $P_{a,zz}$ = + 0.85 ± 0.02)



Theory

A. Abragam: The Principles of Nuclear Magnetism

Hamiltonian to describe the nuclear relaxation of a H_2 molecules

$$\boxed{H = \omega_I (I^1_z + I^2_z) + \omega_J J_z + \omega' (\mathbf{I^1} + \mathbf{I^2})\cdot\mathbf{J} + \omega'' \{ \mathbf{I^1}\cdot \mathbf{I^2} - 3(\mathbf{I^1}\cdot \mathbf{n})(\mathbf{I^2} \cdot \mathbf{n})\}}$$

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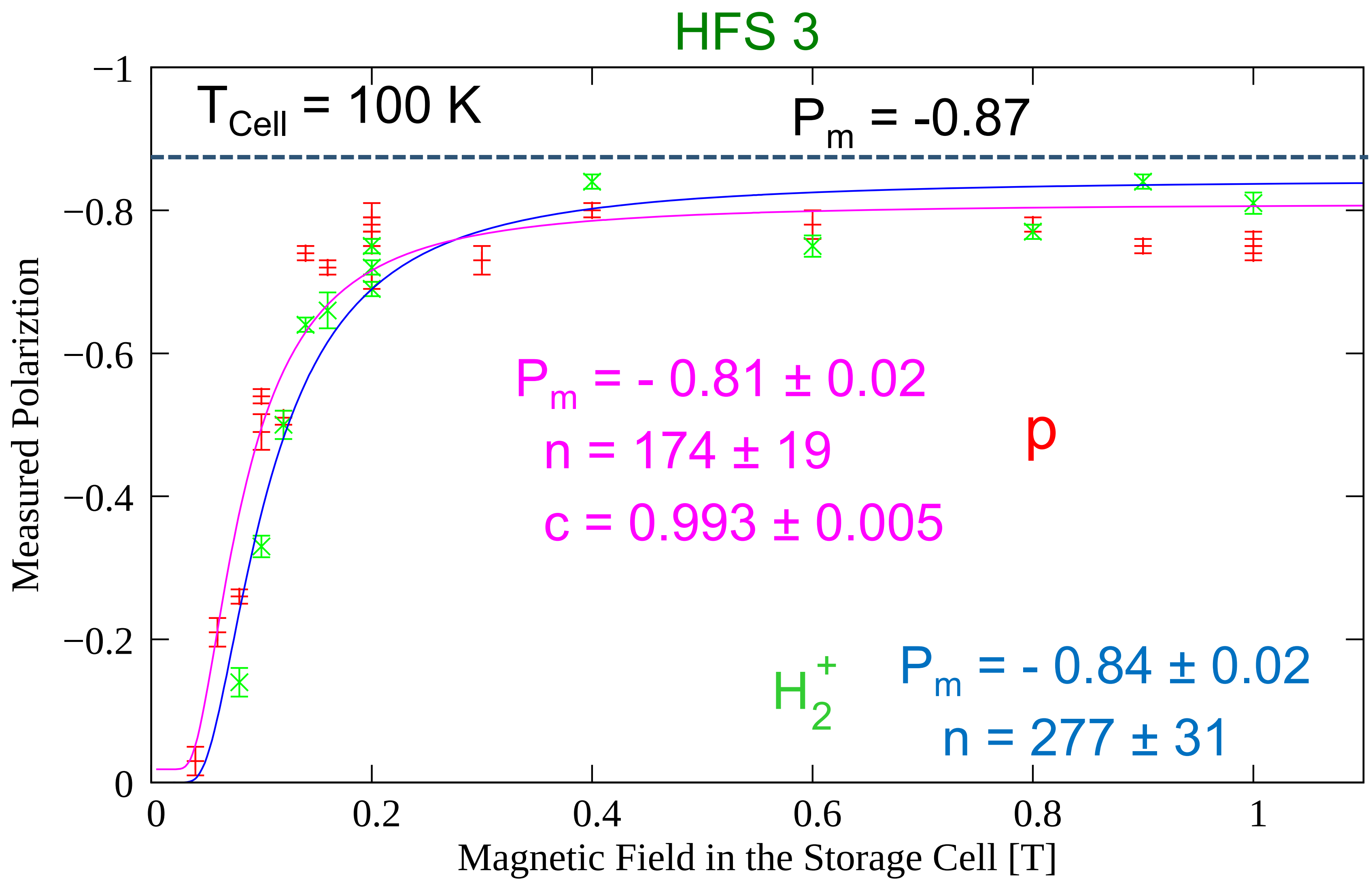
$\omega'' = 2 \gamma_I H'' = \gamma_I^2 \hbar / b^3$ is the strength of the dipolar coupling between the protons, b is their distance, and $\mathbf{n}$ is the unit vector $\mathbf{b}/b$ ($H'' = 3.4$ mT).

$$B_c (H_z) \neq B_c (D_z) \neq B_c (D_{zz})$$

$$\Rightarrow B_c (D_z) = 8\pm1 \text{ mT} \; / \; B_c (D_{zz}) = 11\pm1 \text{ mT}$$

Experimental results

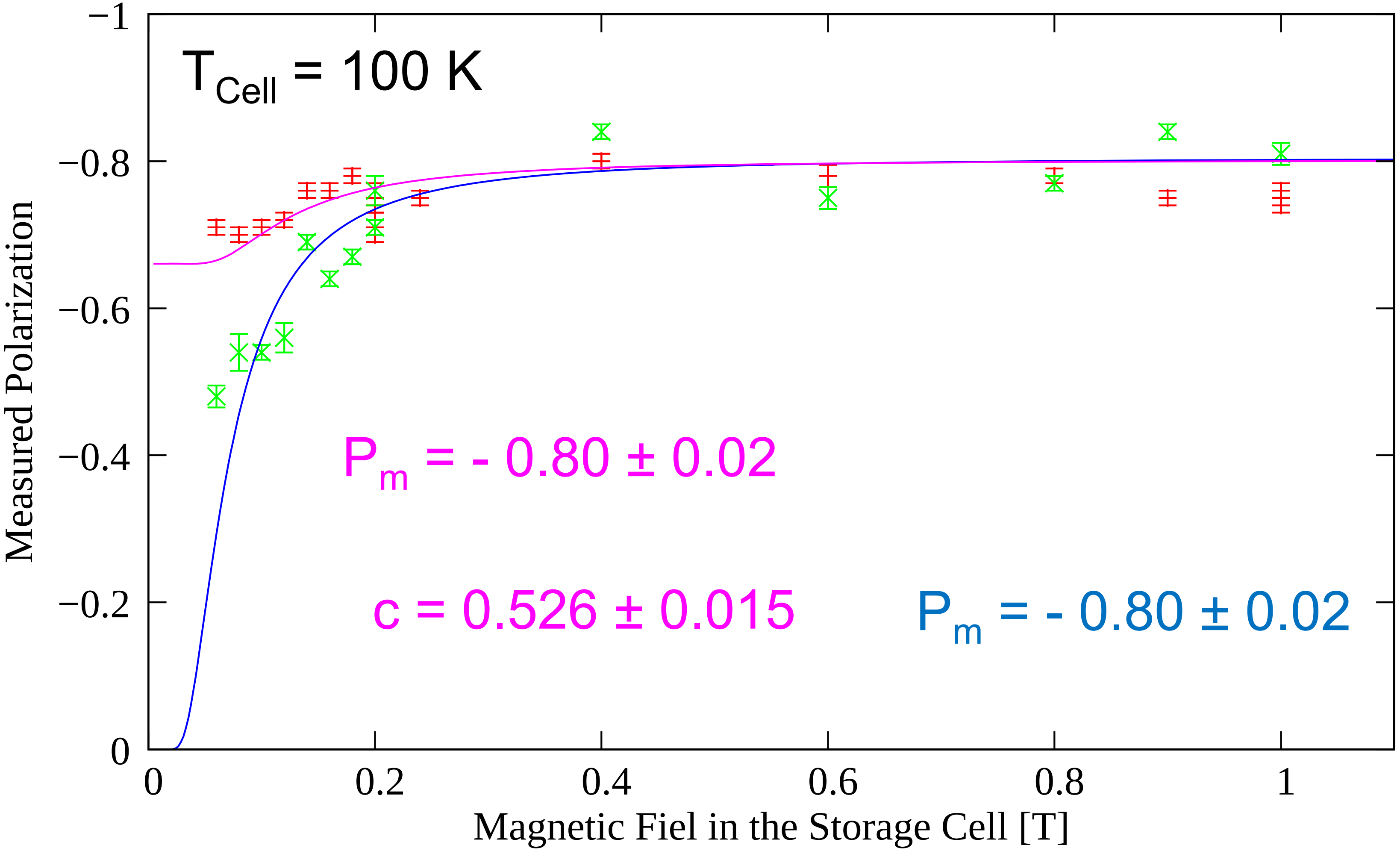
Measurements on Fomblin Oil (Perfluoropolyether PFPE)



Experimental results

Measurements on Fomblin Oil (Perfluorpolyether PFPE)

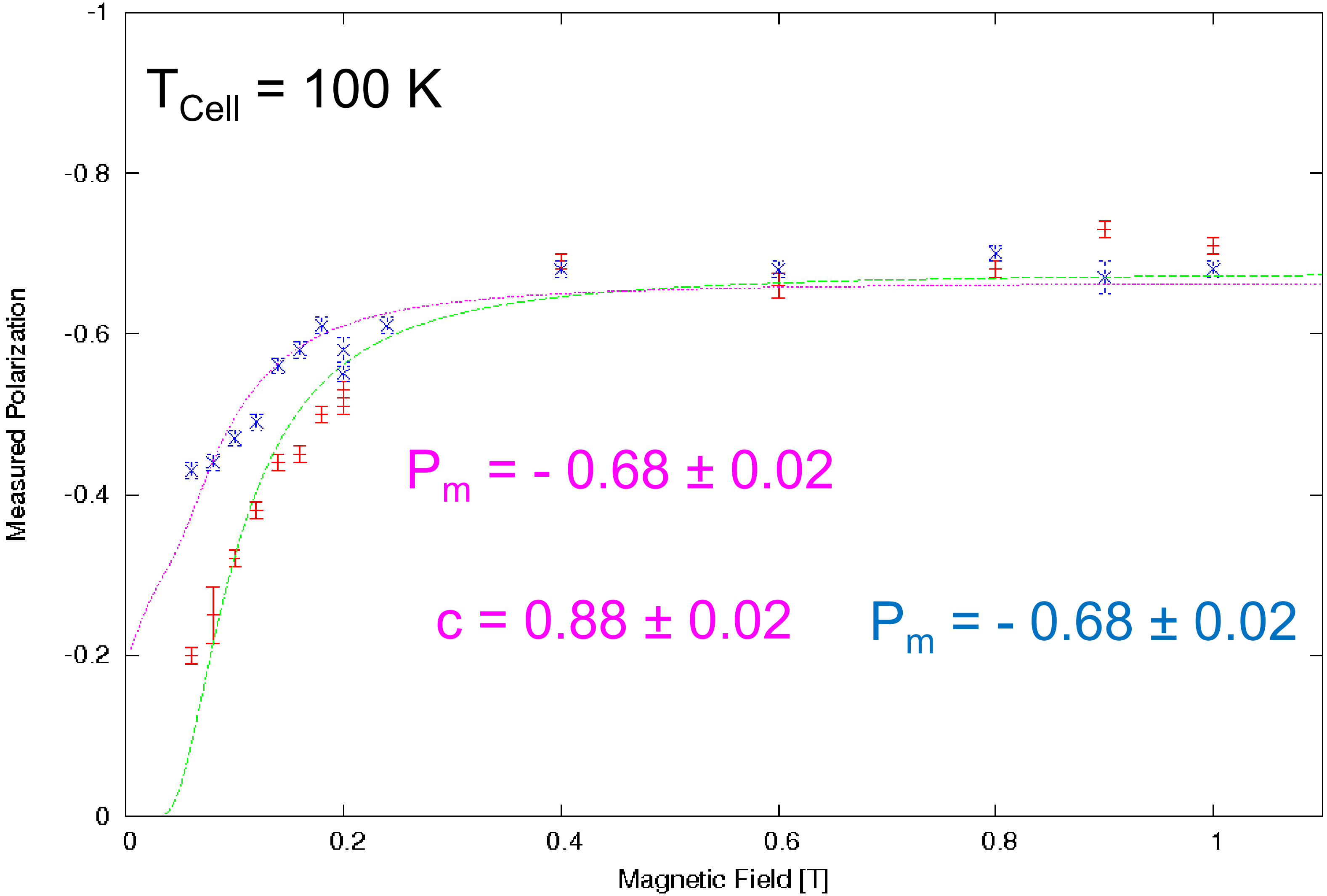
HFS 3: Next attempt



Experimental results

Measurements on Fomblin Oil (Perfluorpolyether PFPE)

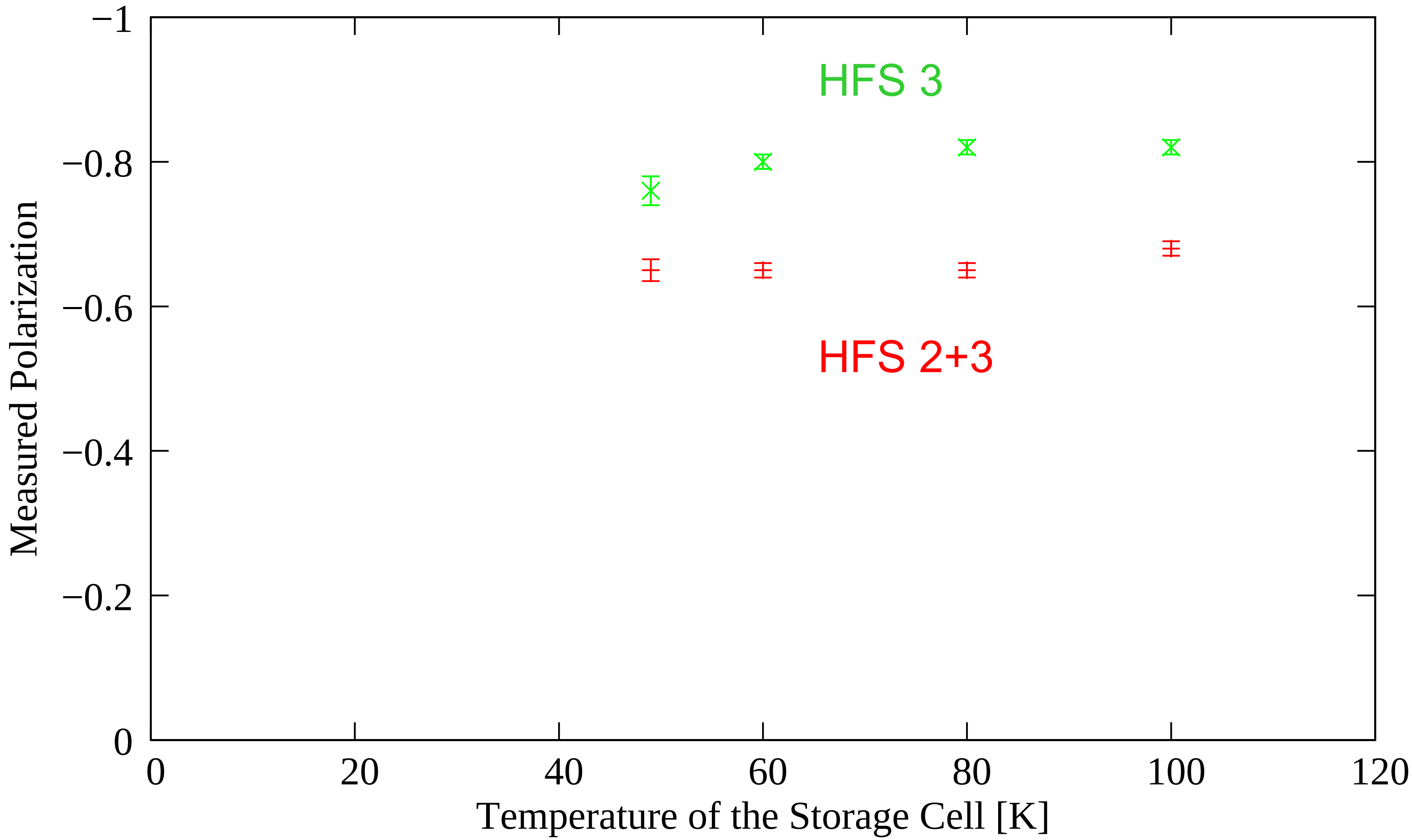
HFS 2+3: Next attempt



Experimental results

Measurements on Fomblin Oil (Perfluorpolyether PFPE)

$B_{cell} = 0.4$ T , H_2^+ only



Conclusion

We can measure:

- the recombination of hydrogen/deuterium atoms on different surfaces, at different temperatures and for different HFS.

- the polarization of atoms and molecules in a storage cell. **=> hyper-polarized H_2/D_2 molecules can be produced !**

- the number of wall collisions of the molecules in the cell. At least, we can see the difference between „hard“ and „soft“ materials (elastic scattering, cos-distribution or $\cos^x$-distribution).

- the B_c for vector- and tensor-polarized Deuterium.

To-do List

- Calculation of B_c for vector- and tensor-polarized Deuterium
- Additional cryo-catcher between ABS and ISTC-chamber
- Measurements on different surfaces:
    - Aluminium
    - Teflon
    - …
- More measurements on a water surface
  (Maybe the surface below has some influence …)
- Polarized Deuterium Fuel for polarized fusion reactors

How to get polarized deuterium fuel?

1.) The production of hyper-polarized deuterium molecules is possible !!!

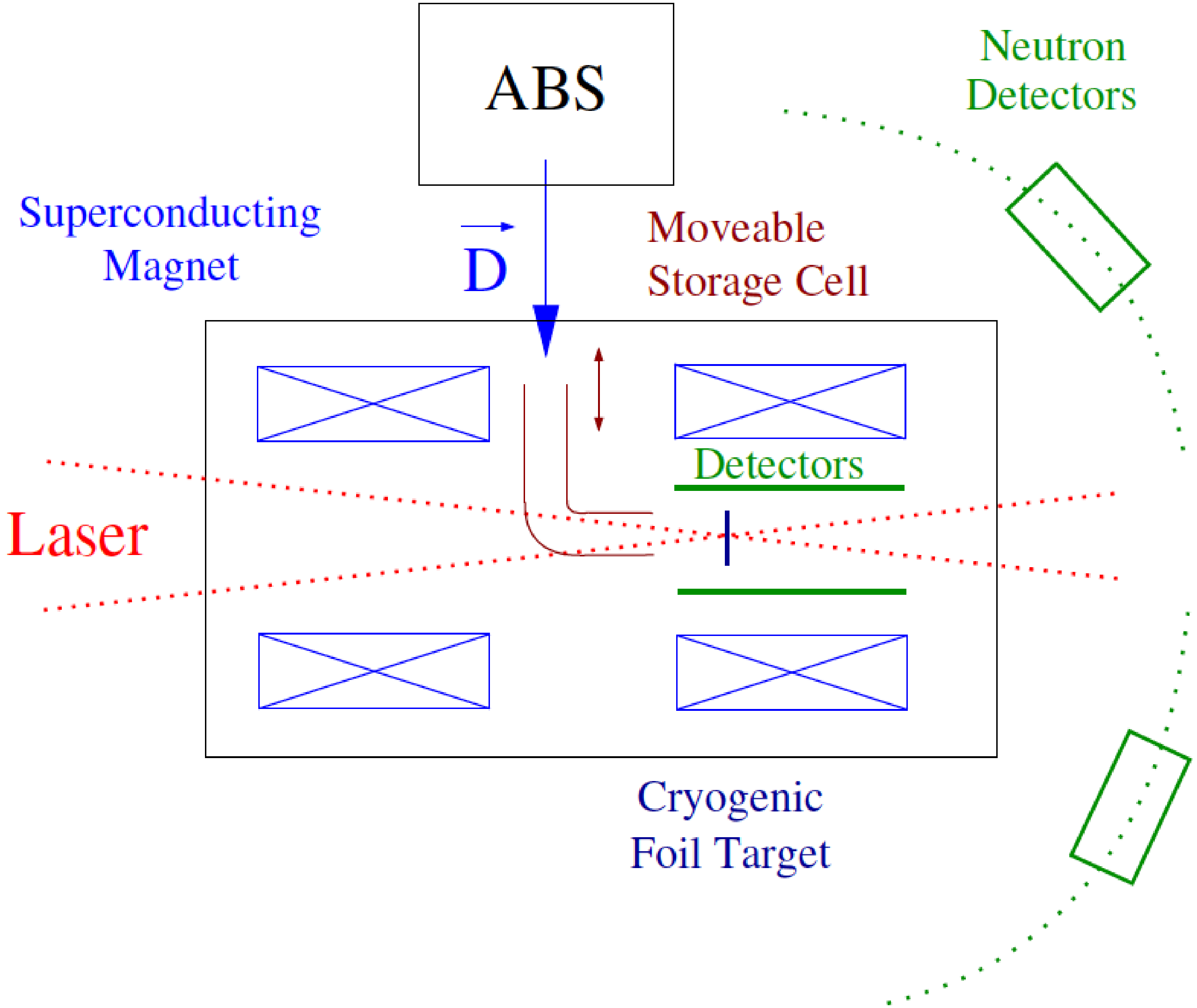
2.) Polarized Deuterium molecules in the gas phase cannot be stored for a long time (~1s at 1T)

3.) The possible amount of polarized Deuterium molecules produced by an ABS cannot exceed 10^{17} molecules/s

But there is hope:

The S=2 state (both nuclear spins parallel) is the ground state
$\Rightarrow$ The deuterium molecules can be cooled further and might be stored and collected to build deuterium ice

Future Ideas



More details in the talk by Markus Büscher

Polarized H_2 Molecules

$\Psi_{a,b}(I, m_I)$ and $I_a = 1,\ I_b = 1$
ortho-deuterium
$\Psi(2,2) = \Psi_a(1,1)\Psi_b(1,1)$
$\Psi(2,1) = \frac{1}{\sqrt{2}}[\Psi_a(1,0)\Psi_b(1,1) + \Psi_a(1,1)\Psi_b(1,0)]$
$\Psi(2,0) = \frac{1}{\sqrt{6}}[\Psi_a(1,1)\Psi_b(1,-1) + 2\Psi_a(1,0)\Psi_b(1,0) + \Psi_a(1,-1)\Psi_b(1,1)]$
$\Psi(2,\text{-}1) = \frac{1}{\sqrt{2}}[\Psi_a(1,0)\Psi_b(1,-1) + \Psi_a(1,-1)\Psi_b(1,0)]$
$\Psi(2,-2) = \Psi_a(1,-1)\Psi_b(1,-1)$
$\Psi(0,0) = \frac{1}{\sqrt{3}}[\Psi_a(1,1)\Psi_b(1,-1) - \Psi_a(1,0)\Psi_b(1,0) + \Psi_a(1,-1)\Psi_b(1,1)]$
para-deuterium
$\Psi(1,1) = \frac{1}{\sqrt{2}}[\Psi_a(1,1)\Psi_b(1,0) - \Psi_a(1,0)\Psi_b(1,1)]$
$\Psi(1,0) = \frac{1}{\sqrt{2}}[\Psi_a(1,+1)\Psi_b(1,-1) - \Psi_a(1,-1)\Psi_b(1,1)]$
$\Psi(1,-1) = \frac{1}{\sqrt{2}}[\Psi_a(1,0)\Psi_b(1,-1) - \Psi_a(1,-1)\Psi_b(1,0)]$

S=0 and S=2 are the groundstates

Outlook: Polarized Fusion

$\vec{t} + \vec{d} \longrightarrow {}^4He + n$ Factor: ~1.5 at 107 keV

${}^3\vec{He} + \vec{d} \longrightarrow {}^4He + p$ Factor: ~1.5 at 430 keV

Advantages:

1.) Increased energy gain (ITER: ~ 2 / Megajoule: ~ 4)
or reduced costs for the reactor

2.) Focussing of the neutrons on special wall areas
or suppression of the neutrons for a neutron lean reactor
($E \sim B^{7.84}$)

Outlook: Polarized Fusion

Problems to solve:

1.) All double-polarized cross sections must be known !

-> d-d reactions are missing

-> Measurements are underway at PNPI

2.) Does the polarization survives in the fusion plasma ?

-> Laser-induced fusion: Test with pol. ^{3}He gas is foreseen in 2016

-> Tokomak: Joined collaboration between Jlab and DIII

3.) How to produce and handle polarized deuterium ?

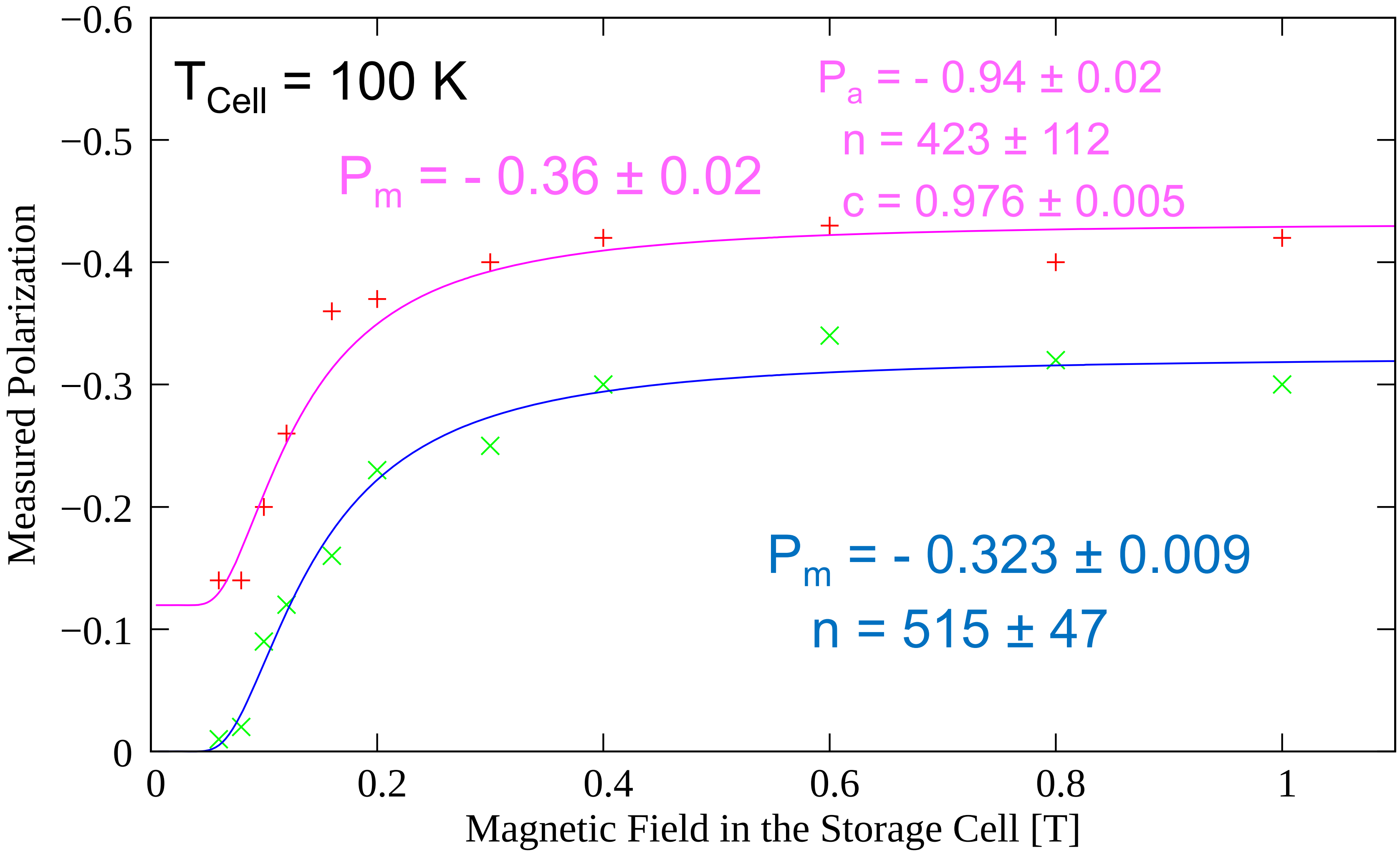
-> maybe pol. Deuterium molecules can be frozen out, collected and stored for some time

Nicolai Tchernov:
First Spokesperson of this ISTC Project

Experimental results

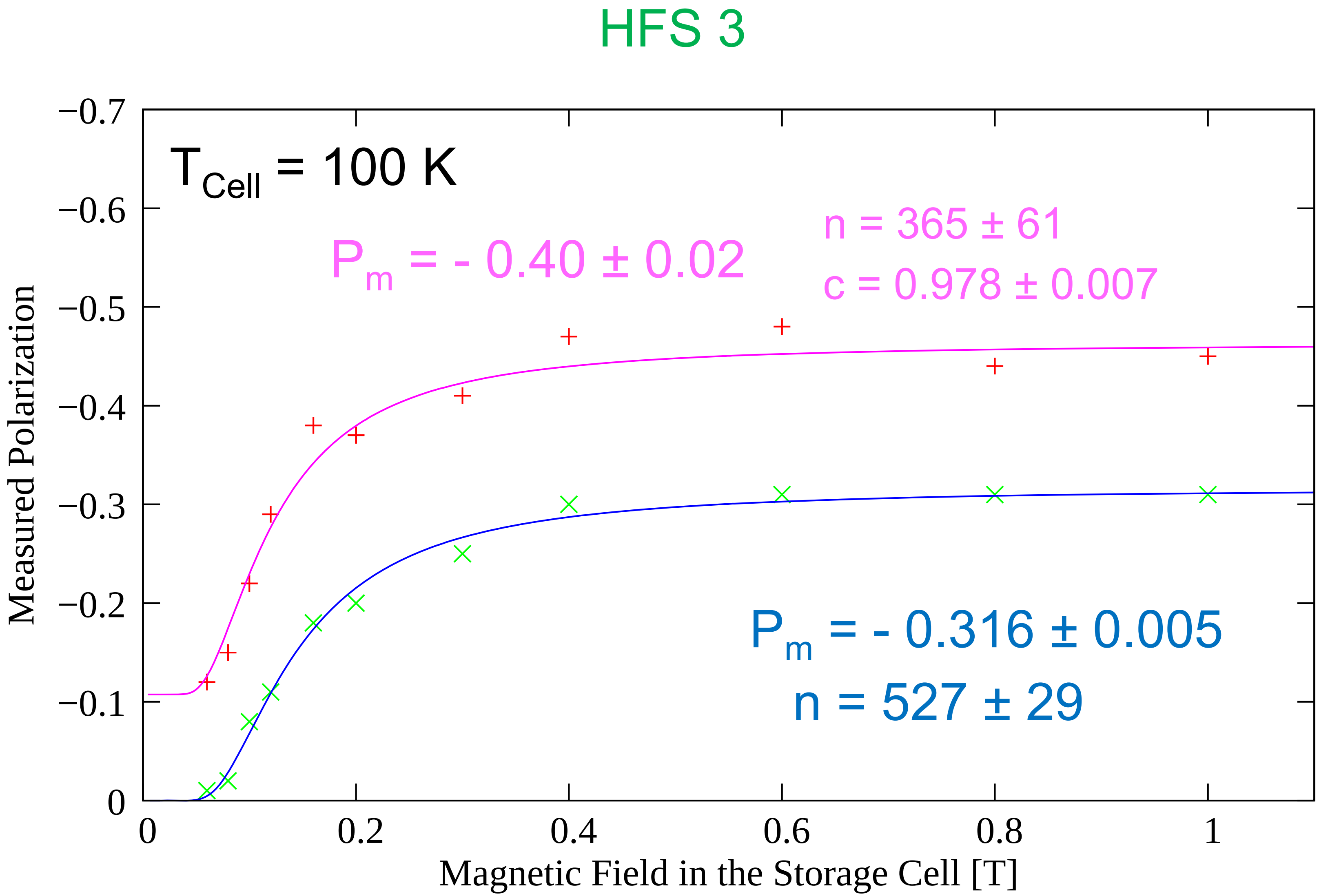
Measurements on Fused Quartz Glass after several days

HFS 2+3



Experimental results

Measurements on Fused Quartz Glass after several days



Experimental results

Measurements on Fomblin Oil (Perfluorpolyether PFPE)